Second Edition

Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Volume I
Introduction and Hydrocarbons

Volume II
Halogenated Hydrocarbons

Volume III
Oxygen Containing Compounds

Volume IV
Nitrogen and Sulfur Containing Compounds and Pesticides

Donald Mackay
Wan Ying Shiu
Kuo-Ching Ma
Sum Chi Lee
Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH, and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the “best” or “right” values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or 25°C. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry’s law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in Chapter 1 how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a “typical” or “generic” or “evaluative” environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.
Acknowledgments

We would never have completed the volumes for the first and second editions of the handbook and the CD-ROMs without the enormous amount of help and support that we received from our colleagues, publishers, editors, friends, and family. We are long overdue in expressing our appreciation.

We would like first to extend deepest thanks to these individuals: Dr. Warren Stiver, Rebecca Lun, Deborah Tam, Dr. Alice Bobra, Dr. Frank Wania, Ying D. Lei, Dr. Hayley Hung, Dr. Antonio Di Guardo, Qiang Kang, Kitty Ma, Edmund Wong, Jenny Ma, and Dr. Tom Harner. During their past and present affiliations with the Department of Chemical Engineering and Applied Chemistry and/or the Institute of Environment Studies at the University of Toronto, they have provided us with many insightful ideas, constructive reviews, relevant property data, computer know-how, and encouragement, which have resulted in substantial improvements to each consecutive volume and edition through the last fifteen years.

Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patricia Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

We are indebted to Brian Lewis, Vivian Collier, Kathy Feinstein, Dr. David Packer, and Randi Cohen for their interest and help in taking our idea of the handbook to fruition.

We also would like to thank Professor Doug Reeve, Chair of the Department of Chemical Engineering and Applied Chemistry at the University of Toronto, as well as the administrative staff for providing the resources and assistance for our efforts.

We are grateful to the University of Toronto and Trent University for providing facilities, to the Natural Sciences and Engineering Research Council of Canada and the consortium of chemical companies that support the Canadian Environmental Modelling Centre for funding of the second edition. It is a pleasure to acknowledge the invaluable contributions of Eva Webster and Ness Mackay.
Biographies

Donald Mackay, born and educated in Scotland, received his degrees in Chemical Engineering from the University of Glasgow. After working in the petrochemical industry he joined the University of Toronto, where he taught for 28 years in the Department of Chemical Engineering and Applied Chemistry and in the Institute for Environmental Studies. In 1995 he moved to Trent University to found the Canadian Environmental Modelling Centre. Professor Mackay’s primary research is the study of organic environmental contaminants, their properties, sources, fates, effects, and control, and particularly understanding and modeling their behavior with the aid of the fugacity concept. His work has focused especially on the Great Lakes Basin; on cold northern climates; and on modeling bioaccumulation and chemical fate at local, regional, continental and global scales.

His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

Wan-Ying Shiu is a Senior Research Associate in the Department of Chemical Engineering and Applied Chemistry, and the Institute for Environmental Studies, University of Toronto. She received her Ph.D. in Physical Chemistry from the Department of Chemistry, University of Toronto, M.Sc. in Physical Chemistry from St. Francis Xavier University, and B.Sc. in Chemistry from Hong Kong Baptist College. Her research interest is in the area of physical-chemical properties and thermodynamics for organic chemicals of environmental concern.

Kuo-Ching Ma obtained his Ph.D. from Florida State University, M.Sc. from The University of Saskatchewan, and B.Sc. from The National Taiwan University, all in Physical Chemistry. After working many years in the aerospace, battery research, fine chemicals, and metal finishing industries in Canada as a Research Scientist, Technical Supervisor/Director, he is now dedicating his time and interests to environmental research.

Sum Chi Lee received her B.A.Sc. and M.A.Sc. in Chemical Engineering from the University of Toronto. She has conducted environmental research at various government organizations and the University of Toronto. Her research activities have included establishing the physical-chemical properties of organochlorines and understanding the sources, trends, and behavior of persistent organic pollutants in the atmosphere of the Canadian Arctic.

Ms. Lee also possesses experience in technology commercialization. She was involved in the successful commercialization of a proprietary technology that transformed recycled material into environmentally sound products for the building material industry. She went on to pursue her MBA degree, which she earned from York University’s Schulich School of Business. She continues her career, combining her engineering and business experiences with her interest in the environmental field.
# Contents

## Volume I

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Aliphatic and Cyclic Hydrocarbons</td>
<td>61</td>
</tr>
<tr>
<td>3</td>
<td>Mononuclear Aromatic Hydrocarbons</td>
<td>405</td>
</tr>
<tr>
<td>4</td>
<td>Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons</td>
<td>617</td>
</tr>
</tbody>
</table>

## Volume II

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Halogenated Aliphatic Hydrocarbons</td>
<td>921</td>
</tr>
<tr>
<td>6</td>
<td>Chlorobenzenes and Other Halogenated Mononuclear Aromatics</td>
<td>1257</td>
</tr>
<tr>
<td>7</td>
<td>Polychlorinated Biphenyls (PCBs)</td>
<td>1479</td>
</tr>
<tr>
<td>8</td>
<td>Chlorinated Dibenzo-p-dioxins</td>
<td>2063</td>
</tr>
<tr>
<td>9</td>
<td>Chlorinated Dibenzofurans</td>
<td>2167</td>
</tr>
</tbody>
</table>

## Volume III

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Ethers</td>
<td>2259</td>
</tr>
<tr>
<td>11</td>
<td>Alcohols</td>
<td>2473</td>
</tr>
<tr>
<td>12</td>
<td>Aldehydes and Ketones</td>
<td>2583</td>
</tr>
<tr>
<td>13</td>
<td>Carboxylic Acids</td>
<td>2687</td>
</tr>
<tr>
<td>14</td>
<td>Phenolic Compounds</td>
<td>2779</td>
</tr>
<tr>
<td>15</td>
<td>Esters</td>
<td>3023</td>
</tr>
</tbody>
</table>

## Volume IV

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>Nitrogen and Sulfur Compounds</td>
<td>3195</td>
</tr>
<tr>
<td>17</td>
<td>Herbicides</td>
<td>3457</td>
</tr>
<tr>
<td>18</td>
<td>Insecticides</td>
<td>3711</td>
</tr>
<tr>
<td>19</td>
<td>Fungicides</td>
<td>4023</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Appendix</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>4133</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>4137</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>4161</td>
</tr>
</tbody>
</table>
5 Halogenated Aliphatic Hydrocarbons

CONTENTS

5.1 List of Chemicals and Data Compilations ................................................................. 924
  5.1.1 Chloroalkanes and chloroalkenes ................................................................. 924
    5.1.1.1 Chloromethane (Methyl chloride) ......................................................... 924
    5.1.1.2 Dichloromethane .................................................................................. 930
    5.1.1.3 Trichloromethane (Chloroform) .............................................................. 939
    5.1.1.4 Tetrachloromethane (Carbon tetrachloride) ............................................ 950
    5.1.1.5 Chloroethane (Ethyl chloride) ............................................................... 960
    5.1.1.6 1,1-Dichloroethane .............................................................................. 966
    5.1.1.7 1,2-Dichloroethane .............................................................................. 975
    5.1.1.8 1,1,1-Trichloroethane ........................................................................... 985
    5.1.1.9 1,1,2-Trichloroethane ........................................................................... 996
    5.1.1.10 1,1,1,2-Tetrachloroethane ................................................................... 1004
    5.1.1.11 1,1,2,2-Tetrachloroethane ................................................................... 1009
    5.1.1.12 Pentachloroethene ............................................................................... 1017
    5.1.1.13 Hexachloroethane ............................................................................... 1021
    5.1.1.14 1-Chloropropane \((n)\)-Propyl chloride) ................................................. 1024
    5.1.1.15 2-Chloropropane .................................................................................. 1028
    5.1.1.16 1,2-Dichloropropane ........................................................................... 1031
    5.1.1.17 1,2,3-Trichloropropane ....................................................................... 1038
    5.1.1.18 1-Chlorobutane \((n)\)-Butyl chloride) .................................................... 1041
    5.1.1.19 2-Chlorobutane .................................................................................... 1045
    5.1.1.20 1-Chloropentane \((n)\)-Amyl chloride) .................................................... 1047
    5.1.1.21 1-Chlorohexane ................................................................................... 1050
    5.1.1.22 1-Chloroheptane ............................................................................... 1054
    5.1.1.23 1-Chlorooctane ................................................................................... 1056
    5.1.1.24 1-Chlorononane .................................................................................. 1059
    5.1.1.25 1-Chlorodecane ................................................................................... 1061
    5.1.1.26 Chloroethene \((Vinyl chloride) .............................................................. 1063
    5.1.1.27 1,1-Dichloroethene .............................................................................. 1070
    5.1.1.28 \textit{cis}-1,2-Dichloroethene ................................................................... 1077
    5.1.1.29 \textit{trans}-1,2-Dichloroethene ................................................................. 1084
    5.1.1.30 Trichloroethylene .................................................................................. 1091
    5.1.1.31 Tetrachloroethylene ............................................................................ 1104
    5.1.1.32 1,3-Dichloropropene .......................................................................... 1115
    5.1.1.33 Chloroprene ......................................................................................... 1117
    5.1.1.34 Hexachlorobutadiene .......................................................................... 1119
    5.1.1.35 Hexachlorocyclopentadiene .................................................................. 1121
  5.1.2 Bromoalkanes and bromoalkenes ...................................................................... 1123
    5.1.2.1 Bromomethane ....................................................................................... 1123
    5.1.2.2 Dibromomethane ................................................................................... 1128
    5.1.2.3 Tribromomethane ................................................................................... 1134
5.1.2.4 Bromoethane (Ethyl bromide) ...................................................... 1139
5.1.2.5 1,2-Dibromoethane ............................................................... 1143
5.1.2.6 1-Bromopropane ................................................................. 1148
5.1.2.7 2-Bromopropane ................................................................. 1152
5.1.2.8 1,2-Dibromopropane ............................................................ 1154
5.1.2.9 1-Bromobutane (n-Butyl bromide) .......................................... 1156
5.1.2.10 1-Bromopentane (n-Amyl bromide) ....................................... 1158
5.1.2.11 1-Bromohexane ................................................................. 1160
5.1.2.12 1-Bromoheptane ............................................................... 1161
5.1.2.13 1-Bromooctane ................................................................. 1162
5.1.2.14 1-Bromodecane ................................................................. 1164
5.1.2.15 1-Bromododecane .............................................................. 1165
5.1.2.16 Bromocyclohexane .............................................................. 1166
5.1.2.17 Vinyl bromide ................................................................. 1167
5.1.3 Iodoalkanes ............................................................................. 1169
5.1.3.1 Iodomethane (Methyl iodide) ................................................ 1169
5.1.3.2 Iodoethane (Ethyl iodide) ...................................................... 1174
5.1.3.3 1-Iodopropane ................................................................. 1178
5.1.3.4 2-Iodopropane ................................................................. 1181
5.1.3.5 1-Iodobutane ................................................................. 1183
5.1.3.6 1-Iodopentane ................................................................. 1185
5.1.4 Mixed halogenated hydrocarbons ............................................. 1186
5.1.4.1 Bromochloromethane .......................................................... 1186
5.1.4.2 Bromodichloromethane ....................................................... 1188
5.1.4.3 Dibromochloromethane ....................................................... 1190
5.1.4.4 Chlorodifluoromethane (HCFC-22) ....................................... 1193
5.1.4.5 Dichlorodifluoromethane (CFC-12) ...................................... 1196
5.1.4.6 Trichlorofluoromethane (CFC-11) ......................................... 1199
5.1.4.7 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113) ..................... 1203
5.1.4.8 1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112) ............... 1207
5.1.5 Fluoroalkanes and fluoroalkenes ............................................ 1209
Fluoromethane
Difluoromethane
Trifluoromethane
Tetrafluoromethane
Chlorofluoromethane
Dichlorofluoromethane
Chlorodifluoromethane (See also Section 5.1.4. Mixed halogenated hydrocarbons)
Chlorotrifluoromethane
Dichlorodifluoromethane (See also Section 5.1.4. Mixed halogenated hydrocarbons)
Trichlorofluoromethane (See also Section 5.1.4. Mixed halogenated hydrocarbons)
Fluoroethane
1,1-Difluoroethane
1,2-Difluoroethane
1,1,1-Trifluoroethane
1,1,2-Trifluoroethane
1,1,2,2-Tetrafluoroethane
1,1,1,2-Tetrafluoroethane
Pentafluoroethane
Hexafluoroethane
1-Chloro-2-fluoroethane
1-Chloro-1,1-difluoroethane
1-Chloro-1,1,2-trifluoroethane
1-Chloro-1,2,2,2-tetrafluoroethane
1-Chloropentafluoroethane
1,1-Dichloro-1-fluoroethane
1,2-Dichloro-1,1-difluoroethane
1,1-Dichlorotrifluoroethane
1,2-Dichloro-1,1,2,2-tetrafluoroethane
1,1-Dichloro-1,2,2,2-tetrafluoroethane
1,1,1-Trichloro-2,2,2-trifluoroethane
1,1,2-Trichloro-1,2,2-trifluoroethane
1,1-Difluorotetrachloroethane
1,1,2,2-Tetrachloro-1,2-difluoroethane
2-Fluoropropane
1,1,2,2,3-Pentafluoropropane
1,1,1,3,3-Pentafluoropropane
1,1,1,2,2-Pentafluoropropane
1,1,1,2,3,3-Hexafluoropropane
1,1,1,3,3,3-Hexafluoropropane
1,1,1,2,3,3,3-Heptafluoropropane
Octafluoropropane
Trichlorotrifluoro propane
1-Chloro-2,2,2-trifluoropropane
Perfluorobutane
Perfluorocyclobutane
Perfluoropentane
Perfluorocyclopentane
Perfluoro-2-methylcyclopentane
Perfluoro-3-methylcyclopentane
Perfluorocyclohexane
Perfluorohexane
Fluoroethene
1,1-Difluoroethene
Tetrafluoroethene
Chlorotrifluoroethene
1,2-Dichloro-1,2-difluoroethene
1,1-Dichloro-2,2-difluoroethene
3-Fluoropropene
Hexafluoropropene

5.2 Summary Tables and QSAR Plots .......................... 1226
5.3 References ................................................. 1237
5.1 LIST OF CHEMICALS AND DATA COMPILATIONS

5.1.1 CHLOROALKANES AND CHLOROALKENES

5.1.1.1 Chloromethane (Methyl chloride)

\[
\begin{align*}
\text{H} & \quad \text{Cl} & \quad \text{H} \\
\text{H} & \quad \text{Cl} & \quad \text{H}
\end{align*}
\]

Common Name: Chloromethane
Synonym: methyl chloride, monochloromethane
Chemical Name: chloromethane
CAS Registry No: 74-87-3
Molecular Formula: CH₃Cl
Molecular Weight: 50.488
Melting Point (°C): −97.7 (Lide 2003)
Boiling Point (°C): −24.09 (Lide 2003)
Density (g/cm³ at 20°C):
- 0.9159 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
- 0.9214, 0.9111 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
- 55.0 (calculated-density, Wang et al. 1992)
- 50.6, 48.8, 54.3, 50.4 (exptl., Tyn and Calus method, Schroeder method, Le Bas method, Reid et al. 1987)
- 50.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
- 6.43 (Riddick et al. 1986)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 7400 (30°C at 1 atm, McGovern 1943)
- 5346 (gravitational method, Glew & Moelwyn-Hughes 1953)
- 6450 (20°C, Dean 1973)
- 7250 (20°C under 101.3 kPa pressure of CH₃Cl, McConnell et al. 1975; Pearson & McConnell 1975)
- 6270, 5380 (20, 25°C literature average at 760 mmHg, Dilling 1977)
- 5325* (summary of literature data, temp range 5–80°C, Horvath 1982)
- 4800 (Dean 1985)
- 6480 (30°C, quoted, Riddick et al. 1986)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 98048* (248.9 K, static-manometer, measured range 191.4–248.9 K, Messerly & Aston 1940)
- 101325* (–24.0°C, summary of literature data, temp range –99.58 to 24.0°C, Stull 1947)
- 559860 (interpolated from graph, temp range –50 to 60°C, McGovern 1943)
- 100800 (Glew & Moelwyn-Hughes 1953)
- 574500 (calculated-Antoine eq., Dreisbach 1959; 1961)
\[
\log (P/mmHg) = 6.99445 – 902.451/(243.63 + t°C); \text{ temp range } –80 \text{ to } 3°C \text{ (Antoine eq. for liquid state, Dreisbach 1959; 1961)}
\]
log (P/mmHg) = 6.99445 – 902.451/(243.60 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1081* (29.43°C, concentration ratio, measured range 29.43–40.59°C, Swain & Thornton 1962)

539300 (20–25°C, calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = log [–0.2185 × 5375.3/(T/K)] + 7.546207; temp range –99 to 137.5°C (Antoine eq., Dean 1985, 1992)

574600, 572800 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 6.98762 – 899.739/(242.921 + t/°C); temp range –69.2 to –23°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/mmHg) = 6.09349 – 948.58/(249.336 + t/°C); temp range –75.2 to 5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/mmHg) = 25.7264 – 1.7503 × 10^3/(T/K) – 6.7151·log (T/K) – 1.2956 × 10^–9·(T/K)^2; temp range 175–416 K (vapor pressure eq., Yaws 1994)

498820 (293.15 K, selected summary of literature data, temp range 175.44–293.15 K, Xiang 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

953*, 957 (distribution ratio, measured range 4–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)

log {H/(mmHg·L/mol)} = 71.005 – 21.656·log (T/K) – 4043.9/(T/K); temp range 277.24–353.23 K (Glew & Moelwyn-Hughes 1953)

1010 (calculated as 1/K AW, CW/CA, reported as exptl., Hine & Mookerjee 1975)

744, 892 (exptl. as per McConnell et al. 1975, calculated-P/C, Neely 1976)

739 (20°C, Pearson & McConnell 1975)

942 (calculated-C_A/C_W, Dilling 1977)

875 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

log (k_H/atm) = 6.93 – 1248.11/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

951, 950 (calculated-P/C, recommended, Mackay & Shiu 1981)

894* (EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)

ln [H/(atm m^3/mol)] = 9.358 – 4215/(T/K), temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)

669 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

867 (computed value, Yaws et al. 1991)

363, 834 (0, 22°C, distilled water, headspace-GC, Elliot & Rowland 1993)

386 (0°C, gas stripping-GC, Moore et al. 1995)

392, 465, 533 (0, 3.0, 6.0°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

ln K_AW = 9.17 – 2982/(T/K), seawater of salinity of 30.4‰, temp range: 0–6°C (Moore et al. 1995)

668 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

743 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

log K_AW = 3.899 – 1292/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{ow}:

0.91 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

0.91 (shake flask, Log P Database, Hansch & Leo 1987)

0.89, 0.936 (calculated-MO, calculated-π substituent const., Bodor et al. 1989)

0.91 (recommended, Sangster 1989)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C:

1.39 (calculated-measured $\gamma^\infty$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.505 (microorganism-water, calculated from $K_{OW}$, Mabey et al. 1982)

Sorption Partition Coefficient, log $K_{OC}$:

0.633 (calculated-$K_{OW}$, Mabey et al. 1982)

0.778 (selected, Jury et al. 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Volatileization: half-life of 27–28 min for initial concentration of 1 mg/L in an open container stirred at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_\text{1/2}(\text{exptl.}) = 27.6$ min, $t_\text{1/2}(\text{calc}) = 0.599$ min, 14.9 min from water (Dilling 1977)

$t_\text{1/2} \sim 2.4$ h from water (estimated, Thomas 1982);

$t_\text{1/2} \sim 120$ d from soil (estimated, Jury et al. 1990).

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3^-$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

$k_{OH} = 4.7 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, bimolecular rate constant (Yung et al. 1975)

$k_{OH} = 8.5 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, bimolecular rate constant with a lifetime $\tau = 0.37$ yr in the troposphere (Cox et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 250–350 K, with a tropospheric lifetime of 1.19 yr (flash photolysis-resonance fluorescence, Davis et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K with lifetime $\tau = 1.19$ yr, measured range 250–350 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altschuller 1980)

$k_{OH} = (3.6 \pm 0.8) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = (4.4 \pm 0.5) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298.4 K, measured range 298–423 K and the calculated $t_\text{1/2} \sim 0.2$ yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)

$k_{OH} = 24.7 \times 10^6$ mol$^{-1}$ s$^{-1}$ at 297 K (flash photolysis-resonance absorption, Paraskevopoulos et al. 1981)

$k_{OH} = 5.0 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 231 d, loss of 0.4% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}^* = (4.35 \pm 0.21) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 293 K, measured range 247–483 K (discharge-flow resonance fluorescence, Jeong & Kaufman, 1982)

$k_{OH}(\text{calc}) = 2.4 \times 10^{10}$ cm$^3$ mol$^{-1}$ s$^{-1}$ at 300 K (Lyman 1982)

$k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and 0.05 M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{OH}^* = 4.36 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}^* = 4.9 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K, measured range 295–800 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k_{NO3} = 9.8 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson 1991)

Hydrolysis: $k = 6.8 \times 10^{-5}$ h$^{-1}$ with hydrolytic $t_\text{1/2} = 417$ d at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979; Mabey et al. 1982);

hydrolysis $k = 2.371 \times 10^{-4}$ h$^{-1}$ with $t_\text{1/2} = 0.93$ yr (Mabey & Mill 1978)

$t_\text{1/2} = 7000$ h, based on neutral and base catalyzed hydrolysis rate constants at 25°C extrapolated from data obtained at higher temperatures (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation:

$t_\text{1/2}(\text{aq. aerobic}) = 668–762$ h, based on unacclimated aerobic aqueous screening test data for dichloromethane from experiments utilizing selected domestic waste water inoculum (Tabak et al. 1981; quoted, Howard et al. 1991) and activated sludge inoculum (Klecka 1982; quoted, Howard et al. 1991);

$t_\text{1/2}(\text{aq. anaerobic}) = 672–2688$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (Darnall et al. 1976); tropospheric lifetime of 1.19 yr due to reaction with OH radical (Davis et al. 1976); estimated residence time to be about 2 yr for the reaction with OH radical in troposphere (Singh et al. 1979); lifetime $\tau = 1.19$ yr for reaction with OH radical (Altshuller 1980); residence time of 231 d, loss of 0.4% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981); estimated residence time in troposphere to be 1 yr (Lyman 1982); $t_{1/2} = 1472–14717$ h, based on photooxidation half-life in air from measured rate constants for reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991); estimated tropospheric lifetimes of 1.3 yr, and 1.54 yr by rigorous calculation (Nimitz & Skaggs 1992); lifetime for reaction with OH radicals, $\tau = 11.7$ yr for Polar region, $\tau = 2.2$ yr for Middle region and $\tau = 0.8$ yr for Tropical region in the Northern hemisphere; $\tau = 0.9$ yr for Tropical, $\tau = 3.6$ yr for Middle and $\tau = 12.3$ yr for Polar region in the Southern hemisphere; $\tau = 1.4$ yr in the Global atmosphere, based on data from 1981–1996 (Khalil & Rasmussen 1999a). Surface water: $t_{1/2} = 168–672$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991). Ground water: $t_{1/2} = 336–1344$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991). Sediment:

Soil: $t_{1/2} > 50$ d (Ryan et al. 1988); estimated $t_{1/2} = 120$ d for volatilization from soil (Jury et al. 1990); $t_{1/2} = 168–672$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991). Biota: $t_{1/2} > 50$ d, subject to plant uptake from soil via volatilization (Ryan et al. 1988).

<table>
<thead>
<tr>
<th>Table 5.1.1.1</th>
<th>Reported aqueous solubilities and Henry’s law constants of chloromethane (methyl chloride) at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>S/(wt%) = 1.4019 – 6.3562 × 10⁻²(t/°C) + 1.71977 × 10⁻³(t/°C)² – 2.8262 × 10⁻⁵(t/°C)³ + 2.5268 × 10⁻⁷(t/°C)⁴ – 9.3470 × 10⁻¹⁰(t/°C)⁵ (1)</td>
<td></td>
</tr>
<tr>
<td><strong>Aqueous solubility</strong></td>
<td><strong>Henry’s law constant</strong></td>
</tr>
<tr>
<td>summary of literature data</td>
<td></td>
</tr>
<tr>
<td>$t$/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>5</td>
<td>14019</td>
</tr>
<tr>
<td>10</td>
<td>9113</td>
</tr>
<tr>
<td>20</td>
<td>6274</td>
</tr>
<tr>
<td>25</td>
<td>5325</td>
</tr>
<tr>
<td>30</td>
<td>4579</td>
</tr>
<tr>
<td>40</td>
<td>3490</td>
</tr>
<tr>
<td>50</td>
<td>2742</td>
</tr>
<tr>
<td>60</td>
<td>2228</td>
</tr>
<tr>
<td>70</td>
<td>1891</td>
</tr>
<tr>
<td>80</td>
<td>1609</td>
</tr>
<tr>
<td>eq.1</td>
<td>S/wt%</td>
</tr>
<tr>
<td>A</td>
<td>59.096</td>
</tr>
<tr>
<td>B</td>
<td>21.656</td>
</tr>
<tr>
<td>C</td>
<td>4043.9</td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for chloromethane.

FIGURE 5.1.1.2 Logarithm of Henry’s law constant versus reciprocal temperature for chloromethane.
TABLE 5.1.1.2
Reported vapor pressures of chloromethane (methyl chloride) at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C\log (T/K) + D(T/K) \quad (5)
\end{align*}
\]

Messerly & Aston 1940

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>191.424</td>
<td>3509</td>
<td>248.998</td>
<td>101521</td>
<td>191.378</td>
<td>3498</td>
</tr>
<tr>
<td>194.556</td>
<td>4474</td>
<td>-92.4</td>
<td>1333</td>
<td>-99.58</td>
<td>666.6</td>
</tr>
<tr>
<td>206.324</td>
<td>10320</td>
<td>31.07167</td>
<td>-76.0</td>
<td>5333</td>
<td></td>
</tr>
<tr>
<td>213.539</td>
<td>16343</td>
<td>1822.60</td>
<td>-70.4</td>
<td>7999</td>
<td></td>
</tr>
<tr>
<td>213.526</td>
<td>16328</td>
<td>9.287119</td>
<td>-63.0</td>
<td>13332</td>
<td></td>
</tr>
<tr>
<td>222.999</td>
<td>28384</td>
<td>0.00555556</td>
<td>-51.2</td>
<td>26664</td>
<td></td>
</tr>
<tr>
<td>230.184</td>
<td>41739</td>
<td>-38.0</td>
<td>53329</td>
<td></td>
<td></td>
</tr>
<tr>
<td>237.125</td>
<td>59004</td>
<td>mp/K</td>
<td>175.44</td>
<td>-24.0</td>
<td>101325</td>
</tr>
<tr>
<td>242.845</td>
<td>77224</td>
<td>bp/K</td>
<td>248.94</td>
<td></td>
<td></td>
</tr>
<tr>
<td>246.441</td>
<td>90805</td>
<td>∆H_v/(kJ mol⁻¹) = 0.945</td>
<td>mp/K</td>
<td>-97.7</td>
<td></td>
</tr>
</tbody>
</table>

Stull 1947

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>-97.7</td>
<td>666.6</td>
</tr>
</tbody>
</table>

Summary of literature data

FIGURE 5.1.1.3 Logarithm of vapor pressure versus reciprocal temperature for chloromethane.
5.1.1.2 Dichloromethane

Common Name: Dichloromethane
Synonym: methylene chloride, methylene dichloride, methane dichloride, methylene bichloride
Chemical Name: dichloromethane
CAS Registry No: 75-09-2
Molecular Formula: CH₂Cl₂
Molecular Weight: 84.933

Melting Point (°C):
-95.2 (Lide 2003)

Boiling Point (°C):
40 (Lide 2003)

Density (g/cm³ at 20°C):
1.3255, 1.3163 (20°C, 25°C, Dreisbach 1959; 1961)
1.3266 (Horvath 1982; Weast 1982–83)
1.3256, 1.131678 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
64.0 (calculated-density, Wang et al. 1992)
71.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
28.56, 28.98 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔHfus (kJ/mol):
1.435 (calculated, Dreisbach 1959; 1961)
1.472 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
20000* (20°C, volumetric method, Rex 1906)
19910 (Seidell 1940)
13200 (25°C, data presented between 0–50°C in graph, McGovern 1943)
34480 (shake flask-residue volume method, Booth & Everson 1948)
13200 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
20000* (Archer & Sterns 1977; Andelman 1978; measured range 0–30°C, quoted, Horvath 1982)
22700, 19400 (1.5, 20°C, literature average, Dilling 1977)
13700 (shake flask-titration/turbidity, Coca et al. 1980)
13030* (summary of literature data, Horvath 1982)
13000 (selected, Thomas 1982; Riddick et al. 1986; Howard 1990)
16700 (Verschueren 1983; selected, Valsaraj 1988)
19020 (calculated-UNIFAC activity coeff., Banerjee 1985)
17200* (26.8°C, shake flask-GC/TC, measured range 0–35.7°C, Stephenson 1992)
19260, 19830, 19500, 19500 (20, 30, 35, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
18080, 19995, 20880, 21850 (20, 30, 35, 40°C, infinite dilution activity coeff. γ-UNIFAC, Tse et al. 1992)
20080, 18800, 18880 (10, 20, 30°C, activity coeff. γ-differential pressure transducer, Wright et al. 1992)
18650 (gas stripping-GC, Li et al. 1993)
20340 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
46510, 68170 (20°C, 30°C, Rex 1906)
57120 (interpolated from graph, temp range –40 to 110°C, McGovern 1943)
Halogenated Aliphatic Hydrocarbons

57480*  (Antoine eq. regression, temp range –70 to 40.3°C, Stull 1947)
58100  (calculated-Antoine eq., Dreisbach 1959; 1961)
\[ \log (P_{\text{mmHg}}) = 7.07138 - 1134.6/(231.0 + t/°C) \]; temp range –28 to 121°C (Antoine eq. for liquid state, Dreisbach 1955)
\[ \log (P_{\text{mmHg}}) = 7.0803 - 1138.91/(231.45 + t/°C) \]; temp range 30–40°C (Antoine eq. from reported exp. data, Boublík et al. 1973)
49704 (calculated-Antoine eq., temp range –70 to 40.7°C, Weast 1972–73)
\[ \log (P_{\text{mmHg}}) = \left[-0.2185 \times 7572.3/(T/\text{K})\right] + 8.18330 \]; temp range –70 to 40.7°C (Antoine eq., Weast 1972–73)
58275, 57270  (calculated-Antoine eq., Boublik et al. 1973)
\[ \log (P_{\text{mmHg}}) = 9.72567 - 2979.516/(395.553 + t/°C) \]; temp range 30–40°C (Antoine eq. from reported exp. data, Boublik et al. 1973)
48200  (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
21065, 57062  (1.5, 25°C, Dow Chemicals data, Dilling 1977)
57950, 57980  (calculated-Antoine eq., Boublik et al. 1984)
\[ \log (P_{\text{mmHg}}) = 5.96841 - 1014.441/(216.227 + t/°C) \]; temp range 30–40°C (Antoine eq. from reported exp. data, Boublík et al. 1984)
47990  (selected, Daniels et al. 1985)
\[ \log (P_{\text{mmHg}}) = 7.4092 - 1325.9/(252.6 + t/°C) \]; temp range –40 to 40°C (Antoine eq., Dean 1985, 1992)
58100  (selected, Riddick et al. 1986)
\[ \log (P_{\text{Pa}}) = 6.07622 - 1070.07/(223.24 + t/°C) \]; temp range not specified (Antoine eq., Riddick et al. 1986)
57990  (calculated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P_{\text{atm}}) = 6.18649 - 1126.53/(–43.46 + T/\text{K}) \]; temp range 264–312 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\[ \log (P_{\text{atm}}) = 6.88926 - 1545.323/(3.375 + T/\text{K}) \]; temp range 311–383 K (Antoine eq.-II, Stephenson & Malanowski 1987)
\[ \log (P_{\text{atm}}) = 5.87285 - 861.817/(–94.102 + T/\text{K}) \]; temp range 379–455 K (Antoine eq.-III, Stephenson & Malanowski 1987)
\[ \log (P_{\text{atm}}) = 5.20540 - 449.586/(–193.701 + T/\text{K}) \]; temp range 450–510 K (Antoine eq., Stephenson & Malanowski 1987)
47660, 71000, 102540  (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
\[ \log (P_{\text{mmHg}}) = 32.5069 - 2.5166 \times 10^3/(T/\text{K}) - 8.8015 \log (T/\text{K}) + 1.2934 \times 10^{-10} \times (T/\text{K})^2; \]
temp range 178–510 K (vapor pressure eq., Yaws 1994)
57844  (selected summary of literature data, temp range 178.25–338.15 K, Xiang 2002)
70486  (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
231.3  (calculated as 1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}, reported as exp., Hine & Mookerjee 1975)
301.0  (McConnell et al. 1975; Pearson & McConnell 1975)
322.3  (calculated, Neely 1976)
292, 271.5  (exp., calculated-C_{\text{W}}/C_{\text{A}}, Dilling 1977)
111.3  (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
\[ \log (k_{\text{H}}/\text{atm}) = 7.92 - 1821.84/(T/\text{K}) \] (least-square regression of data from lit., Kavanaugh & Trussell 1980)
295  (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
295*  (24.9°C equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C Leighton & Calo 1981)
\[ \ln (k_{\text{H}}/\text{atm}) = 17.42 - 3645/(T/\text{K}) \]; temp range 1.9–24.9°C (equilibrium cell-concn ratio measurements, Leighton & Calo 1981)
205.7  (calculated-P/C, Mabey et al. 1982)
303.9  (calculated-P/C, Thomas 1982)
229.1  (20°C, EPICS-GC, Lincoff & Gossett 1983)
227.9  (20°C, EPICS-GC, Lincoff & Gossett 1984)
\[ \ln \left[ \frac{H}{(\text{atm m}^3/\text{mol})} \right] = 8.200 - 4191/(T/\text{K}) \; \text{temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)} \]
\[ \ln \left[ \frac{H}{(\text{atm m}^3/\text{mol})} \right] = 9.035 - 4472/(T/\text{K}) \; \text{temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)} \]
\[ \ln \left[ \frac{H}{(\text{atm m}^3/\text{mol})} \right] = 9.843 - 5612/(T/\text{K}) \; \text{temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)} \]
\[\text{Octanol/Water Partition Coefficient, log } K_{OW} \text{ at 25°C or as indicated. Additional data at other temperatures designated with an asterisk are compiled at the end of this section:} \]
\[1.25 \] (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
\[1.51 \] (Hansch & Leo 1979)
\[1.22 \] (HPLC-\(k'\) correlation, Hafkenscheid & Tomlinson 1983)
\[1.25 \] (HPLC-\(k'\) correlation, Tomlinson & Hafkenscheid 1986)
\[1.25 \] (recommended, Sangster 1989)
\[1.35 \] (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
\[1.25 \] (recommended, Hansch et al. 1995)
\[1.25 \] (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

\[\text{Octanol/Air Partition Coefficient, log } K_{OA} \text{ at 25°C:} \]
\[2.27 \] (head-space GC, Abraham et al. 2001)

\[\text{Bioconcentration Factor, log } BCF: \]
\[0.699 \] (calculated as per Lyman et al. 1982, Howard 1990)
\[0.778 \] (microorganism-water, calculated from \(K_{OW}\), Mabey et al. 1982)
\[0.600 \] (calculated-MCI \(\chi\), Koch 1983)
\[0.362 \] (selected, Daniels et al. 1985)

\[\text{Sorption Partition Coefficient, log } K_{OC}: \]
\[0.944 \] (calculated-\(K_{OW}\), Mabey et al. 1982)
\[1.440 \] (calculated- MCI \(\chi\), Koch 1983; quoted, Bahnick & Doucette 1988)
\[1.000 \] (selected, Daniels et al. 1985)
\[1.390 \] (calculated-MCI \(\chi\), Bahnick & Doucette 1988)

\[\text{Sorption Partition Coefficient, log } K_{OM}: \]
\[1.44, 1.23 \] (quoted, calculated-MCI \(\chi\), Sabljic 1984)
Environmental Fate Rate Constants, and Half-Lives, \( t_{1/2} \):

Volatilization: \( t_{1/2}(\text{calc}) = 2.23 \text{ min} \) (Mackay & Wolkoff 1973; quoted, Dilling et al. 1975; Callahan et al. 1979); \( t_{1/2}(\text{calc}) = 20.7 \text{ min} \) (Mackay & Leinonen 1975; quoted, Dilling 1977; Callahan et al. 1979); \( t_{1/2}(\text{exptl}) = (21 \pm 3) \text{ min} \) for 1 ppm in water at 25°C when stirred at 200 rpm in water (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982); evaporation \( t_{1/2}(\text{exptl}) = (18.3–25.2) \text{ min} \), \( t_{1/2}(\text{calc}) = 2.23 \) and \( 20.7 \text{ min} \) at 25°C and \( t_{1/2}(\text{exptl}) = 34.9 \text{ min} \), \( t_{1/2} = 24.5 \text{ min} \) at 1.5°C (Dilling 1977); \( t_{1/2} \approx 3.0 \text{ h} \) from water (estimated, Thomas 1982); \( t_{1/2} \approx 100 \text{ d} \) from soil (estimated, Jury et al. 1990).

Photolysis: estimated photodecomposition \( t_{1/2} > 250 \text{ h} \) from a simulated environmental sunlight exposure (> 290 nm at 27 ± 1°C) study (Dilling et al. 1976; quoted, Callahan et al. 1979); photodegradation \( t_{1/2} = 30–120 \text{ d} \) (Darnall et al. 1976; quoted, Daniels et al. 1985); photocatalyzed mineralization by the presence of TiO\(_2\) with a rate of 1.6 ppm/min per gram of catalyst (Ollis 1985).

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\) or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{\text{OH}} = 1.24 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K corresponding to a lifetime of 0.30 yr} \text{ (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)}
\]

\[
k_{\text{OH}*} = (1.16 \pm 0.05) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K with lifetime of 0.39 yr, measured range 245–375 K} \text{ (flash photolysis-resonance fluorescence, Davis et al. 1976)}
\]

\[
k_{\text{OH}} = 1.55 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \text{ (discharge flow-LMR, Howard & Evenson 1976a)}
\]

\[
k_{\text{OH}} = (14.5 \pm 2.0) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298.5 K and the calculated tropospheric half-life of \approx 0.05 yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)}
\]

\[
k_{\text{OH}} = 1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ residence time of 77 d, loss of 1.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)}
\]

\[
k_{\text{OH}*} = 1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 292 K, measured range 251–455 K (discharge flow-resonance fluorescence, Jeong & Karfman 1982)}
\]

\[
k < 360 \text{ M}^{-1} \text{ h}^{-1} \text{ for singlet oxygen and 0.2 M}^{-1} \text{ h}^{-1} \text{ for peroxy radical at 25°C (Mabey et al. 1982)}
\]

\[
k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1} \text{ for reaction with O}_3 \text{ in water as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)}
\]

\[
\text{photooxidation } t_{1/2} = 458–4584 \text{ h based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)}
\]

\[
k = 4.0 \times 10^{7} \text{ M}^{-1} \text{ s}^{-1} \text{ with reference to CH}_3\text{CCl}_3 \text{ (Buxton et al. 1988; quoted, Haag & Yao 1992)}
\]

\[
k_{\text{OH}} = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k(\text{soln}) = 9.6 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)}
\]

\[
k_{\text{OH}*} = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989)}
\]

\[
k_{\text{OH}} = 1.76 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K, measured range 298–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)}
\]

\[
k = (9 \pm 6) \times 10^{7} \text{ M}^{-1} \text{ h}^{-1} \text{ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)}
\]

Hydrolysis: a minimum hydrolysis \( t_{1/2} = 18 \text{ months} \) was estimated from aqueous reactivity experiments (Dilling et al. 1975; quoted, Callahan et al. 1979; Howard 1990); rate constant \( k = 3.2 \times 10^{-11} \text{ s}^{-1} \) with a maximum \( t_{1/2} = 704 \text{ yr} \) for hydrolysis at pH 7 and 25°C was reported from the extrapolated experimental data obtained at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

\[
t_{1/2} = 260000 \text{ d in natural waters at pH 7 (Capel & Larson 1995)}
\]

Biodegradation: completely biodegradable under aerobic conditions with sewage seed or activated sludge between 6 h to 7 d (Rittman & McCarty 1980; Davis et al. 1981; Tabak et al. 1981; Klecka 1982; Stover & Kincannon 1983; quoted, Howard 1990)

\[
t_{1/2}(\text{aq. aerobic}) = 168–672 \text{ h based on unacclimated aerobic screening test data (Kawasaki 1980; Tabak et al. 1981; quoted, Howard et al. 1991); \( t_{1/2}(\text{aq. anaerobic}) = 672–2688 \text{ h based on unacclimated aerobic biodegradation half-life (Howard et al. 1991)}
\]

\[
t_{1/2}(\text{aerobic}) = 7 \text{ d}, \ t_{1/2}(\text{anaerobic}) = 28 \text{ d in natural waters (Capel & Larson 1995)}
\]

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 33$ wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 2.4$–$24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

lifetime of 4.4 yr in troposphere for the reaction with OH radical (Altshuller 1980)

estimated disappearance time to be 12 h to 1.0 year in simulated troposphere chamber (Dilling & Goersch 1979; quoted, Lyman 1982)

residence time of 77 d, loss of 1.3% in 1d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time in troposphere to be 160–250 d (Lyman 1982);

$S/(wt\%) = 1.961 - 4.4883 \times 10^{-2}(t/°C) + 8.6617 \times 10^{-4}(t/°C)^2 + 4.9463 \times 10^{-6}(t/°C)^3$ (1)

1. Rex 1906 volumetric method

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>23630</td>
</tr>
<tr>
<td>10</td>
<td>21220</td>
</tr>
<tr>
<td>20</td>
<td>20000</td>
</tr>
<tr>
<td>30</td>
<td>19690</td>
</tr>
</tbody>
</table>

Andelman 1978

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>23100</td>
</tr>
<tr>
<td>10</td>
<td>20800</td>
</tr>
<tr>
<td>20</td>
<td>19600</td>
</tr>
<tr>
<td>30</td>
<td>20000</td>
</tr>
</tbody>
</table>

Horvath 1982 summary of literature data

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>19610</td>
</tr>
<tr>
<td>10</td>
<td>15938</td>
</tr>
<tr>
<td>20</td>
<td>13702</td>
</tr>
<tr>
<td>30</td>
<td>13030</td>
</tr>
</tbody>
</table>

Stephenson 1992 shake flask-GC

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>19200</td>
</tr>
<tr>
<td>10</td>
<td>19200</td>
</tr>
<tr>
<td>20</td>
<td>18000</td>
</tr>
<tr>
<td>30</td>
<td>17700</td>
</tr>
</tbody>
</table>

Soil: $t_{1/2} = 10$–$50$ d (Ryan et al. 1988);

volatilization $t_{1/2} \sim 100$ d from soil (Jury et al. 1990);

biodegradation $t_{1/2}(\text{aerobic}) = 1.3$ d (0.16 ppm, conc of dichloromethane), $t_{1/2} = 9.4$ d (0.5 ppm), $t_{1/2} = 191.4$ d (5 ppm), all in sandy loam soil; $t_{1/2} = 54.8$ d in sand (0.5 ppm); $t_{1/2} = 12.7$ d (0.5 ppm) in sandy clay loam soil; $t_{1/2} = 7.2$ d (0.5 ppm) in clay with 50 d lag and $t_{1/2}(\text{anaerobic}) = 21.5$ d (5 ppm) with 70 d lag (Davis & Madsen 1991);

$S/(wt\%) = 1.961 - 4.4883 \times 10^{-2}(t/°C) + 8.6617 \times 10^{-4}(t/°C)^2 + 4.9463 \times 10^{-6}(t/°C)^3$ (1)

1. Rex 1906

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>23630</td>
</tr>
<tr>
<td>10</td>
<td>21220</td>
</tr>
<tr>
<td>20</td>
<td>20000</td>
</tr>
<tr>
<td>30</td>
<td>19690</td>
</tr>
</tbody>
</table>

Andelman 1978

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>23100</td>
</tr>
<tr>
<td>10</td>
<td>20800</td>
</tr>
<tr>
<td>20</td>
<td>19600</td>
</tr>
<tr>
<td>30</td>
<td>20000</td>
</tr>
</tbody>
</table>

Horvath 1982 summary of literature data

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>19610</td>
</tr>
<tr>
<td>10</td>
<td>15938</td>
</tr>
<tr>
<td>20</td>
<td>13702</td>
</tr>
<tr>
<td>30</td>
<td>13030</td>
</tr>
</tbody>
</table>

Stephenson 1992 shake flask-GC

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g.m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>19200</td>
</tr>
<tr>
<td>10</td>
<td>19200</td>
</tr>
<tr>
<td>20</td>
<td>18000</td>
</tr>
<tr>
<td>30</td>
<td>17700</td>
</tr>
</tbody>
</table>

Biota: $t_{1/2} = 10$–$50$ d, subject to plant uptake in soil via volatilization (Ryan et al. 1988);

t$_{1/2} = 0.4$–$0.5$ d to eliminate from small fish (McCarty et al. 1992).
TABLE 5.1.1.2.1 (Continued)

2.

<table>
<thead>
<tr>
<th>Tse et al. 1992</th>
<th>Wright et al. 1992</th>
</tr>
</thead>
<tbody>
<tr>
<td>activity coefficient</td>
<td>activity coefficient</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>20</td>
<td>19260</td>
</tr>
<tr>
<td>30</td>
<td>19830</td>
</tr>
<tr>
<td>35</td>
<td>19500</td>
</tr>
<tr>
<td>40</td>
<td>19500</td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.2

Reported vapor pressures of dichloromethane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/°C) \quad (2) \quad \ln P = A - B/(C + t/°C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log P = A - B/(T/K) - C\log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Mueller &amp; Ignatoswski 1960</th>
<th>Boublik 1960, thesis</th>
</tr>
</thead>
<tbody>
<tr>
<td>summary of literature data</td>
<td>in Boublík et al. 1984</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>–70.0</td>
<td>133.3</td>
<td>29.993</td>
</tr>
<tr>
<td>–52.1</td>
<td>666.6</td>
<td>34.993</td>
</tr>
<tr>
<td>–43.3</td>
<td>1333</td>
<td>38.993</td>
</tr>
<tr>
<td>–33.4</td>
<td>2666</td>
<td>39.993</td>
</tr>
<tr>
<td>–22.3</td>
<td>5333</td>
<td>6.230</td>
</tr>
<tr>
<td>–15.7</td>
<td>7999</td>
<td>9.457</td>
</tr>
<tr>
<td>–6.30</td>
<td>13332</td>
<td>13.289</td>
</tr>
</tbody>
</table>
TABLE 5.1.1.2.2 (Continued)

<table>
<thead>
<tr>
<th>Summary of Literature Data</th>
<th>Mueller &amp; Ignatoswski 1960</th>
<th>Boulik 1960, Thesis in Boulik et al. 1984</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>8.0</td>
<td>26664</td>
<td>16.693</td>
</tr>
<tr>
<td>24.1</td>
<td>53329</td>
<td>21.199</td>
</tr>
<tr>
<td>40.7</td>
<td>101325</td>
<td>26.393</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–96.7</td>
<td>32.337</td>
</tr>
<tr>
<td></td>
<td></td>
<td>39.429</td>
</tr>
</tbody>
</table>

eq. 2 P/kPa
A 6.18791
B 127.232
C 229.764
bp 39.767

FIGURE 5.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for dichloromethane.
TABLE 5.1.1.2.3
Reported Henry's law constants of dichloromethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{T/K} \quad (1) \\
\ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} \quad (2) \\
\ln H = A - \frac{B}{T/K} \quad (3) \\
K_{AW} = A - B \cdot \left( \frac{T}{K} \right) + C \cdot \left( \frac{T}{K} \right)^2 \quad (5)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>equilibrium cell-GC</td>
<td>EPICS-GC</td>
<td>EPICS-GC</td>
<td>activity coefficient</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( H/(Pa , m^3/mol) )</td>
<td>( H/(Pa , m^3/mol) )</td>
<td>( H/(Pa , m^3/mol) )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>1.9</td>
<td>112</td>
<td>9.6</td>
<td>116.5</td>
<td>10</td>
</tr>
<tr>
<td>13.5</td>
<td>203</td>
<td>17.5</td>
<td>132.7</td>
<td>15</td>
</tr>
<tr>
<td>15.7</td>
<td>222</td>
<td>24.8</td>
<td>221.9</td>
<td>20</td>
</tr>
<tr>
<td>22.0</td>
<td>286.5</td>
<td>34.6</td>
<td>330.3</td>
<td>25</td>
</tr>
<tr>
<td>24.9</td>
<td>295</td>
<td>eq. 3</td>
<td>295.3</td>
<td>30</td>
</tr>
<tr>
<td>25</td>
<td>eq. 4</td>
<td>( H/(atm , m^3/mol) )</td>
<td>6.653</td>
<td>eq. 4 *</td>
</tr>
<tr>
<td>eq. 3</td>
<td>( k_H/atm )</td>
<td>B</td>
<td>4215</td>
<td>A</td>
</tr>
<tr>
<td>A</td>
<td>17.42</td>
<td></td>
<td></td>
<td>B</td>
</tr>
<tr>
<td>B</td>
<td>3645</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for dichloromethane.
### TABLE 5.1.1.2.4
Reported octanol-water partition coefficients of dichloromethane at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.35</td>
</tr>
<tr>
<td>35</td>
<td>1.34</td>
</tr>
<tr>
<td>50</td>
<td>1.37</td>
</tr>
</tbody>
</table>

enthalpy of transfer
\[ \Delta H/(kJ \ mol^{-1}) = -20.2 \]

\[ \log K_{OW} = A - \Delta H/2.303RT \]

<table>
<thead>
<tr>
<th>A</th>
<th>\Delta H</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0195</td>
<td>-20.2</td>
</tr>
</tbody>
</table>

#### FIGURE 5.1.1.2.4
Logarithm of K_{OW} versus reciprocal temperature for dichloromethane.
5.1.1.3 Trichloromethane (Chloroform)

Common Name: Trichloromethane
Synonym: chloroform, trichloromethane
Chemical Name: trichloromethane
CAS Registry No: 67-66-3
Molecular Formula: CHCl₃
Molecular Weight: 119.378

Melting Point (°C):
-63.41 (Lide 2003)

Boiling Point (°C):
61.17 (Lide 2003)

Density (g/cm³ at 20°C):
1.4832 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.49845, 1.48911, 1.47970 (15, 20, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
80.0 (calculated-density, Mailhot 1987; Wang et al. 1992)
92.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
33.35, 29.37 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔHfus (kJ/mol):
8.80 (calculated, Dreisbach 1959)
9.54 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
8220, 7760 (20°C, 30°C, volumetric method, Rex 1906)
8520, 7710 (15, 30°C, shake flask-interferometer, Gross & Saylor 1931)
8000 (Wright & Schaffer 1932)
7361 (Seidell 1940)
7700 (Seidell 1941)
7900 (data presented from 0–50°C in graph, McGovern 1943)
13320 (shake flask-residue volume method, Booth & Everson 1948)
8000 (20°C, Stephen & Stephen 1963)
8150 (20°C, Riddick & Bunger 1970)
8200 (20°C, Pearson & McConnell 1975)
8000 (20°C, Neely 1976; Verschueren 1977)
10300, 7840 (1.5, 25°C, selected, Dilling 1977)
7230 (shake flask-LSC, Banerjee et al. 1980)
11900 (shake flask-titration/turbidity, Coca et al. 1980)
7360 (shake flask-LSC, Veith et al. 1980)
7920* (summary of literature data, temp range 0–60°C, Horvath 1982)
2525 (30°C, headspace-GC, McNally & Grob 1984)
7190 (calculated-UNIFAC activity coeff., Banerjee 1985)
8200 (shake flask-radiometric method, Lo et al. 1986)
8150 (20°C, selected, Riddick et al. 1986)
8080, 7435, 7290 (20, 35, 50°C, infinite dilution activity coeff. γ–GC, Barr & Newsham 1987)
8670 (23–24°C, shake flask-GC, Broholm et al. 1992)
8200*, 7900 (19.6°C, 29.5°C, shake flask-GC/TC, measured range 0–59.2°C, Stephenson 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21115, 31990 (20°C, 30°C, Rex 1906)
39345* (35.0°C, vapor-liquid equilibrium, measured range 35.0–60.0°C, Scatchard & Raymond 1938)
26660 (interpolated from graph, temp range –30 to 170°C, McGovern 1943)
25700* (interpolated-Antoine eq. regression, temp range –58.0 to 61.3°C, Stull 1947)
26310 (calculated-Antoine eq., Dreisbach 1959)

\[ \log (P/\text{mmHg}) = 6.90328 - \frac{1163.0}{227.0 + t/°C}; \text{ temp range –15 to 90°C} \]

\[ \log (P/\text{mmHg}) = 6.93708 - \frac{1171.2}{227.0 + t/°C}; \text{ temp range –13 to 97°C} \]

23080 (interpolated from Antoine eq., temp range –58 to 254°C, Weast 1972–73)

log (P/\text{mmHg}) = \left[ -0.2185 \times 7500.5/(T/K) \right] + 7.735083; \text{ temp range –58 to 254°C} (Antoine eq., Weast 1972–73)
26240, 18950 (calculated-Antoine eq., Boublik et al. 1973)

log (P/\text{mmHg}) = 6.85465 – 1170.966/(226.252 + t/°C); \text{ temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)}

log (P/\text{mmHg}) = 6.4934 – 959.44/(196.03 + t/°C); \text{ temp range (Antoine eq. from reported exptl. data, Boublík et al. 1973)}

26217, 26104 (static method-differential pressure gauge, Bissell & Williamson 1975)
20000 (20°C, Pearson & McConnell 1975)
25590 (literature average, Dilling 1977)
21330 (20°C, Verschuuren 1983)

26220, 32080 (calculated-Antoine eq., Boublík et al. 1984)
21330 (20°C, quoted, McNally & Grob 1984)

\[ \log (P/\text{kPa}) = 5.96288 – 1106.94/(218.552 + t/°C); \text{ temp range not specified} \]

log (P/kPa) = 6.4934 – 929.44/(196.03 + t/°C); \text{ temp range –36 to 61°C} (Antoine eq., Dean 1985, 1992)
25970 (selected, Riddick et al. 1986)

log (P/kPa) = 5.96288 – 1106.94/(218.552 + t/°C); \text{ temp range (Antoine eq., Riddick et al. 1986)}
26220 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.07853 – 1170.42/(–46.98 + T/K); \text{ temp range 262–334 K} (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 5.38327 – 948.979/(–61.73 + T/K); \text{ temp range 227–269 K} (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.11152 – 1173.606/(–48.54 + T/K); \text{ temp range 333–416 K} (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 7.89882 – 2879.244/(–161.978 + T/K); \text{ temp range 410–481 K} (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/kPa) = 4.58922 – 181.802/(–325.74 + T/K); \text{ temp range 479–523 K} (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 56.6178 – 3.2462 \times 10^1/(T/K) – 18.7 \log (T/K) + 9.515 \times 10^3-(T/K) + 1.1553 \times 10^{-12}\times(T/K)^2; \text{ temp range 210–536 K (vapor pressure eq., Yaws 1994)}

26182 (selected summary of literature data, temp range 209.64–368.15 K, Xiang 2002)
32408 (30°C, vapor-liquid equilibrium VLE data, Pathare et al. 2004)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

314.1 (20°C, Dilling et al. 1975)
440.8 (calculated as 1/K_{AW}, C_W/C_A, Hine & Mookerjee 1975)
283.4 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
310 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log \( (k_d/\text{atm}) = 9.10 - 2103.09/(T/K) \) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

373* (equilibrium cell-conc ratio-GC/FID, Leighton & Calo 1981)

ln \( (k_d/\text{atm}) = 18.97 - 4046/(T/K) \) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

292.0 (20°C, calculated-P/C, Mabey et al. 1982; Mills et al. 1982)

536.9 (batch stripping-GC, Munz & Roberts 1982; Roberts & Dändliker 1983; Roberts et al. 1985)

432.2 (calculated-UNIFAC activity coeff., Arbuckle 1983)

ln \( K_{AW} = 10.63 - 3649/(T/K) \); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith et al. 1983)

298 (calculated-P/C, Jury et al. 1984; Jury et al. 1990)

337.4; 308 (20°C, EPICS-GC; batch air stripping-headspace GC, Lincos & Gossett 1984)

ln \( [H/(\text{atm m}^3/\text{mol})] = 8.553 - 4180/(T/K) \); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)

304; 486, 365 (20°C, batch air stripping-GC; calculated-P/C; quoted lit. values, Nicholson et al. 1984)

334, 294, 314 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

411 (computed value, Yaws et al. 1991)

199.3* (26.5°C, tap water, EPICS-GC, measured range 26.5–47.2°C, Tancrède & Yanagisawa 1990)

log \( K_{AW} = 4.990 - 1729/(T/K) \), temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

177, 444 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)

126, 214, 352 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

K_{AW} = 0.0394 + 0.00486·(T/K); temp range 0–60°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)

312 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)

331.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

370.8 (modified EPICS method-GC, Ryu & Park 1999)

411; 260 (EPICS-GC; calculated-P/C, David et al. 2000)

307 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log \( K_{AW} = 5.343 - 1830/(T/K) \) (summary of literature data, Staudinger & Roberts 2001)

704.5 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

408* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

ln \( K_{AW} = 10.96 - 3821.3/(T/K) \); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)
Octanol/Water Partition Coefficient, log $K_{ow}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.97</td>
<td>(Hansch &amp; Anderson 1967)</td>
</tr>
<tr>
<td>1.97</td>
<td>(shake flask-UV, Hansch et al. 1968; Leo et al. 1971; Hansch et al. 1975)</td>
</tr>
<tr>
<td>1.94</td>
<td>(Hansch &amp; Leo 1979)</td>
</tr>
<tr>
<td>1.90</td>
<td>(shake flask-LSC, Banerjee et al. 1980)</td>
</tr>
<tr>
<td>1.90</td>
<td>(shake flask-LSC, Veith et al. 1980)</td>
</tr>
<tr>
<td>1.81</td>
<td>(HPLC-k’ correlation, McDuffie 1981)</td>
</tr>
<tr>
<td>2.15</td>
<td>(HPLC-k’ correlation, Wells et al. 1981)</td>
</tr>
<tr>
<td>1.91</td>
<td>(calculated-UNIFAC activity coeff., Arbuckle 1983)</td>
</tr>
<tr>
<td>1.90</td>
<td>(HPLC-k’ correlation, Hafkenscheid &amp; Tomlinson 1983)</td>
</tr>
<tr>
<td>2.14, 2.13, 2.03</td>
<td>(HPLC-k’ correlation, Tomlinson &amp; Hafkenscheid 1986)</td>
</tr>
<tr>
<td>1.66</td>
<td>(calculated-UNIFAC activity coeff., Banerjee &amp; Howard 1988)</td>
</tr>
<tr>
<td>1.97</td>
<td>(recommended, Sangster 1989)</td>
</tr>
<tr>
<td>2.00*</td>
<td>(infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia &amp; Sandler 1995)</td>
</tr>
<tr>
<td>1.86*</td>
<td>(24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.80</td>
<td>(equilibrium head-space-GC, Abraham et al. 2001)</td>
</tr>
<tr>
<td>2.55; 2.53</td>
<td>(equilibrium headspace-GC; calculated-$K_{ow}$/$K_{aw}$, Batterman et al. 2002)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.92</td>
<td>(calculate-$K_{ow}$, Veith et al. 1979; quoted, Veith et al. 1980)</td>
</tr>
<tr>
<td>0.78</td>
<td>(bluegill sunfish, Barrows et al. 1980; Bysshe 1982)</td>
</tr>
<tr>
<td>0.78</td>
<td>(bluegill sunfish, Veith et al. 1980; Veith &amp; Kosian 1982; quoted, Davies &amp; Dobbs 1984; Suntio et al. 1988; Isnard &amp; Lambert 1988; Saito et al. 1992)</td>
</tr>
<tr>
<td>0.63</td>
<td>(calculated-$K_{ow}$, Mackay 1982)</td>
</tr>
<tr>
<td>1.41</td>
<td>(microorganisms-water, calculated from $K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>0.97</td>
<td>(calculated-MCI $\chi$, Koch 1983)</td>
</tr>
<tr>
<td>0.78</td>
<td>(bluegill sunfish, LSC, Davies &amp; Dobbs 1984)</td>
</tr>
<tr>
<td>2.84</td>
<td>(green algae, Mailhot 1987)</td>
</tr>
<tr>
<td>2.84</td>
<td>($Selenastrum capricornutum$, Mailhot 1987)</td>
</tr>
<tr>
<td>0.52–1.01; 0.204–0.40; 0.46–0.49; 0.552–0.57</td>
<td>(rainbow trout; bluegill sunfish; large mouth bass; catfish, Howard 1990)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log $K_{oc}$ at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.64</td>
<td>(calculated-$K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>1.65</td>
<td>(calculated-MCI $\chi$, Koch 1983)</td>
</tr>
<tr>
<td>2.15</td>
<td>(wastewater solids with correlation to $K_{ow}$, Dobbs et al. 1989)</td>
</tr>
<tr>
<td>1.44</td>
<td>(20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)</td>
</tr>
<tr>
<td>1.98</td>
<td>(20°C, weathered shale, mudrock, sorption isotherm-headspace method, Grathwohl 1990)</td>
</tr>
<tr>
<td>2.79</td>
<td>(20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)</td>
</tr>
<tr>
<td>1.85, 1.92</td>
<td>(20°C, calculated-$K_{ow}$, Grathwohl 1990)</td>
</tr>
<tr>
<td>1.53</td>
<td>(soil, Howard 1990)</td>
</tr>
<tr>
<td>1.46</td>
<td>(selected, Jury et al. 1990)</td>
</tr>
<tr>
<td>1.57; 1.46; 1.54</td>
<td>(Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)</td>
</tr>
<tr>
<td>1.63, 1.65, 1.63, 1.69, 1.65, 1.70</td>
<td>(2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{oc} = 4.12%$, EPICS-GC/FID, Dewulf et al. 1999)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log $K_{om}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.65, 1.40</td>
<td>(quoted, calculated-MCI $\chi$, Sabljic 1984)</td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatileization: calculated $t_{1/2} = 1.4$ min (Mackay & Wolkoff 1973);

primary transport process from the aquatic environment with $t_{1/2} = 21–26$ min at pH 7 and 25°C stirred at 200 rpm in an open container (Dilling et al. 1975)

evaporation rate $k_{(exp)} = 13.2 \times 10^{-5} \text{ g cm}^{-2} \text{ s}^{-1}$ to still air (Chiu & Freed 1977; Chiu et al. 1980)

evaporation $t_{1/2}(\text{calc}) = 1.46$, 2.37 min at 20–25°C, $t_{1/2}(\text{exp}) = 34.6$ min at 1.5°C (Dilling 1977)

$t_{1/2} = 3–5.6$ h for different laboratory studies of evaporation from water with moderate mixing conditions (Smith et al. 1980; Rathbun & Tai 1981; Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} = 1.2$ d in Rhine River and $t_{1/2} = 31$ d in a lake in Rhine Basin (Zoeteman et al. 1980).

$t_{1/2} = 3.7$ h from water (estimated, Thomas 1982);

$t_{1/2} = 29$ min–1.13 d from rivers and streams, calculated using published $O_2$ reaeration values; and

$t_{1/2}(\text{calc}) = 31.2$ h from rivers and streams, calculated using estimated $O_2$ reaeration rate constant (Kaczmar et al. 1984);

predicted $t_{1/2} = 36$ h in a river, $t_{1/2} = 40$ h in a pond and $t_{1/2} = 9–10$ d in a lake (USEPA 1984; quoted, Howard 1990);

$t_{1/2} = 4$ h at 20°C was predicted from a model river of 1 m deep at flowing speed of 1 m/s with a wind velocity of 3 m/s and its Henry’s law constant (Smith et al. 1980; quoted, Howard 1990);

Photolysis: not important only by UV in the stratosphere (Robbins 1976);

probably not significant in aquatic systems (Callahan et al. 1979);

photocatalyzed mineralization by the presence of TiO$_2$ with a rate of 4.4 ppm min$^{-1}$ g$^{-1}$ of catalyst (Ollis 1985).

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with $O_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = 1.14 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime of 0.56 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

troposphere with $t_{1/2} = 0.19–0.32$ yr due to reaction with OH radical (Callahan et al. 1979)

$k_{OH} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}^* = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 249–487 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1982)

$k_{OH} = 6.6 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ of estimated at 300 K (Lyman 1982)

$t_{1/2} = 78.5–3140$ yr from the rate constant for the reaction with OH radical (estimated, Dorfman & Adams 1973)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and 0.7 M$^{-1}$ h$^{-1}$ for peroxo radical both at 25°C (Mabey et al. 1982) $k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation $t_{1/2} = 26–260$ d, based on measured data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k = 4.0 \times 10^{7} \text{ M}^{-1} \text{ s}^{-1}$ with reference to CH$_3$CCl$_3$ (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{OH} = 1.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{(soln)} = 1.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 1.03 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k = (5.4 \pm 3.0) \times 10^{7} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

$k_{OH}^* = 1.03 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: first-order rate constant $k = 0.045 \text{ mo}^{-1}$ with $t_{1/2} \sim 15$ months (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 6.9 \times 10^{-12} \text{ s}^{-1}$ (Radding 1976);

hydrolysis rate constant $k = 6.9 \times 10^{-12} \text{ s}^{-1}$ with $t_{1/2} = 3500$ yr at 25°C and pH 7 (Mabey & Mill 1978).

no hydrolysis in acidic aqueous solutions, and rate constant in alkaline aqueous solution, $k = 0.23 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C, and $k = 2.5 \times 10^{-9} \text{ M}^{-1} \text{ h}^{-1}$ at 25°C in neutral aqueous solutions (Mabey & Mill 1978; Mabey et al. 1982; Mills et al. 1982).
probably not a significant fate process with $t_{1/2} = 3500$ yr, based on reported rate constant $k = 6.9 \times 10^{-12}$ s$^{-1}$ at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Haque et al. 1980).

**Biodegradation:** very slow by BOD bottle experiments (Pearson & McConnell 1975);
- $t_{1/2}$(aq. aerobic) = 4 wk to 6 months by unacclimated screening tests (Kawasaki 1980; Flathman & Dahlgran 1982; quoted, Howard et al. 1991);
- $t_{1/2}$(aq. anaerobic) = 1–4 wk by unacclimated anaerobic screening tests (Bouwer et al. 1981; Bouwer & McCarty 1983; quoted, Howard et al. 1991);
- $k = 0.5$ d$^{-1}$ (Tabak et al. 1981; Mills et al. 1982).

**Bioaccumulation:** weak to moderate bioaccumulation; no evidence of biomagnification of trichloromethane in marine food chain (Callahan et al. 1979).

**Half-Lives in the Environment:**

- **Air:** tropospheric $t_{1/2} = 23$ wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
- disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); residence time of 1.7 yr in troposphere, based on one compartment nonsteady state model (Singh et al. 1978; quoted, Lyman 1982);
- residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981); estimated residence time in N. troposphere to be 100 d (Lyman 1982).
- $t_{1/2} = 623–6231$ h, based on photooxidation half-life in air from measured reaction data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);
- tropospheric lifetime ~ 0.17 yr (estimated, Nimitz & Skaggs 1992).

- **Surface water:** not important for aqueous phase (Dilling et al. 1975);
- $t_{1/2} = 1.0–31$ d in various location in the Netherlands in case of a first order reduction process (estimated, Zoeteman et al. 1980);
- $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

- **Ground water:** $t_{1/2} = 1344–43200$ h, based on unacclimated aqueous aerobic biodegradation and grab sample data of aerobic soil from a ground water aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).
- **Soil:** $t_{1/2} = 10–50$ d (Ryan et al. 1988);
- $t_{1/2} = 100$ d, estimated volatilization loss from soil (Jury et al. 1990);
- disappearance $t_{1/2} = 4.1$ d was calculated from first order kinetic for volatilization loss from soil mixtures (Anderson et al. 1991);
- $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).
- **Biota:** $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);
- $t_{1/2} = 10–50$ d, subject plant uptake via volatilization (Ryan et al. 1988).
TABLE 5.1.1.3.1
Reported aqueous solubilities of trichloromethane at various temperatures

\[
S/(\text{wt}) = 0.995 - 1.0531 \times 10^{-2} \cdot t/°C + 7.9819 \times 10^{-5} \cdot (t/°C)^2 + 6.6431 \times 10^{-7} \cdot (t/°C)^3
\]  

(1)

1.

<table>
<thead>
<tr>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8220</td>
<td>15</td>
<td>8520</td>
<td>0</td>
<td>9905</td>
<td>20</td>
<td>8080</td>
</tr>
<tr>
<td>30</td>
<td>7760</td>
<td>30</td>
<td>7710</td>
<td>10</td>
<td>8983</td>
<td>35</td>
<td>7435</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>7920</td>
<td>20</td>
<td>8216</td>
<td>50</td>
<td>7290</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>7689</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>40</td>
<td>7440</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>50</td>
<td>7511</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>7940</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10200</td>
<td>20</td>
<td>7200</td>
<td>20</td>
<td>7108</td>
</tr>
<tr>
<td>9.5</td>
<td>9300</td>
<td>30</td>
<td>8118</td>
<td>35</td>
<td>7030</td>
</tr>
<tr>
<td>19.6</td>
<td>8200</td>
<td>35</td>
<td>8558</td>
<td>50</td>
<td>7694</td>
</tr>
<tr>
<td>29.5</td>
<td>7900</td>
<td>40</td>
<td>9011</td>
<td></td>
<td></td>
</tr>
<tr>
<td>39.3</td>
<td>7400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>49.2</td>
<td>7700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>59.2</td>
<td>7900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for trichloromethane.
TABLE 5.1.1.3.2
Reported vapor pressures of trichloromethane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C\log (T/K)
\end{align*}
\]

(1) \hspace{1cm} \text{ln } P = A - B/(T/K) \hspace{1cm} (1a)

(2) \hspace{1cm} \text{ln } P = A - B/(C + t/°C) \hspace{1cm} (2a)

(3) \hspace{1cm} \text{ln } P = A - B/(C + T/K)

(4) \hspace{1cm} \text{ln } P = A - B/(T/K) - C\log (T/K)

Scatchard & Raymond 1938

Stull 1947

Boublik & Aim 1972

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>39345</td>
<td>-58.0</td>
<td>133.3</td>
<td>-10.356</td>
<td>4524</td>
<td>46.583</td>
<td>61295</td>
</tr>
<tr>
<td>40.0</td>
<td>48023</td>
<td>-39.1</td>
<td>666.6</td>
<td>-2.610</td>
<td>6967</td>
<td>53.070</td>
<td>77125</td>
</tr>
<tr>
<td>45.0</td>
<td>57800</td>
<td>-29.7</td>
<td>1333</td>
<td>2.882</td>
<td>9306</td>
<td>60.319</td>
<td>98412</td>
</tr>
<tr>
<td>50.0</td>
<td>69218</td>
<td>-19.0</td>
<td>2666</td>
<td>8.010</td>
<td>12046</td>
<td></td>
<td></td>
</tr>
<tr>
<td>55.0</td>
<td>82372</td>
<td>-7.10</td>
<td>5333</td>
<td>11.927</td>
<td>14549</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60.0</td>
<td>97342</td>
<td>0.50</td>
<td>7999</td>
<td>16.417</td>
<td>17921</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.4</td>
<td>13332</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6.07945</td>
<td></td>
</tr>
<tr>
<td>25.9</td>
<td>26664</td>
<td>24.598</td>
<td>25780</td>
<td>A</td>
<td>1170.902</td>
<td></td>
<td></td>
</tr>
<tr>
<td>42.7</td>
<td>53329</td>
<td>28.118</td>
<td>29923</td>
<td>B</td>
<td>226.224</td>
<td></td>
<td></td>
</tr>
<tr>
<td>61.3</td>
<td>101325</td>
<td>32.289</td>
<td>35493</td>
<td>C</td>
<td>36.223</td>
<td>41470</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m.p/°C</td>
<td>-65.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for trichloromethane.
### Table 5.1.1.3.3
Reported Henry’s law constants of trichloromethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{(T/K)} \quad (1) \quad \log K_{AW} = A - \frac{B}{(T/K)} \quad (1a)
\]

\[
\ln \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{(T/K)} \quad (2) \quad \log \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{(T/K)} \quad (2a)
\]

\[
\ln (k_H/\text{atm}) = A - \frac{B}{(T/K)} \quad (3)
\]

\[
\ln H = A - \frac{B}{(T/K)} \quad (4) \quad \log H = A - \frac{B}{(T/K)} \quad (4a)
\]

\[
K_{AW} = A - B \cdot \frac{T}{(K)} + C \cdot \frac{T^2}{(K)^2} \quad (5)
\]

#### 1.

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.90</td>
<td>125.7</td>
<td>9.6</td>
<td>152</td>
<td>10</td>
<td>174</td>
<td>26.5</td>
<td>199.3</td>
</tr>
<tr>
<td>13.5</td>
<td>234.7</td>
<td>17.5</td>
<td>249.3</td>
<td>15</td>
<td>236</td>
<td>27.4</td>
<td>274.9</td>
</tr>
<tr>
<td>15.7</td>
<td>267.6</td>
<td>24.8</td>
<td>371.9</td>
<td>20</td>
<td>336</td>
<td>28.9</td>
<td>401.8</td>
</tr>
<tr>
<td>17.1</td>
<td>282.7</td>
<td>34.6</td>
<td>570.5</td>
<td>25</td>
<td>427</td>
<td>28.9</td>
<td>276.2</td>
</tr>
<tr>
<td>22.0</td>
<td>354.7</td>
<td>57.4</td>
<td>624.8</td>
<td>30</td>
<td>561</td>
<td>29.7</td>
<td>226.6</td>
</tr>
<tr>
<td>24.9</td>
<td>373.5</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>30</td>
<td>561</td>
<td>29.9</td>
<td>277.2</td>
</tr>
<tr>
<td>25</td>
<td>373</td>
<td>A</td>
<td>9.843</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>382.2</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>4612</td>
<td>A</td>
<td></td>
<td>11.41</td>
<td>35.6</td>
<td>693.1</td>
</tr>
</tbody>
</table>

#### 2.

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>306</td>
<td>2</td>
<td>116</td>
<td>10</td>
<td>212</td>
<td>2</td>
<td>108</td>
</tr>
<tr>
<td>35</td>
<td>592</td>
<td>6</td>
<td>135.1</td>
<td>20</td>
<td>341</td>
<td>6</td>
<td>151.3</td>
</tr>
<tr>
<td>50</td>
<td>1046</td>
<td>10</td>
<td>165.7</td>
<td>18.2</td>
<td>276.1</td>
<td>10</td>
<td>181.3</td>
</tr>
<tr>
<td></td>
<td>18.2</td>
<td>25</td>
<td>379.3</td>
<td>0</td>
<td>126</td>
<td>16</td>
<td>297.8</td>
</tr>
<tr>
<td></td>
<td>18.2</td>
<td>25</td>
<td>379.3</td>
<td>10</td>
<td>214</td>
<td>25</td>
<td>407.5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>20</td>
<td>352</td>
<td>35</td>
<td>526.5</td>
<td>35</td>
<td>526.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>352</td>
<td>35</td>
<td>526.5</td>
<td>40</td>
<td>769.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>352</td>
<td>35</td>
<td>526.5</td>
<td>50</td>
<td>1120</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>451</td>
<td>60</td>
<td>1497</td>
<td>60</td>
<td>1497</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>451</td>
<td>60</td>
<td>1497</td>
<td>60</td>
<td>1497</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
FIGURE 5.1.1.3.3 Logarithm of Henry’s law constant versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.4

<table>
<thead>
<tr>
<th>Relative GC-RT Technique</th>
<th>Dewulf et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>log K_{OW}</td>
</tr>
<tr>
<td>25</td>
<td>2.00</td>
</tr>
<tr>
<td>35</td>
<td>2.01</td>
</tr>
<tr>
<td>50</td>
<td>2.00</td>
</tr>
</tbody>
</table>

enthalpy of transfer

\[ \Delta H/(kJ \text{ mol}^{-1}) = -20.2 \]

\[ \log K_{OW} = A - \Delta H/2.303RT \]

\[ A = 1.0195 \]

\[ \Delta H = -20.2 \]

change in enthalpy:

\[ \Delta H_{OW}/(kJ \text{ mol}^{-1}) = 4.2 \]

(=4.4 to 12.8)

enthalpy of transfer

\[ \Delta H_{oct}/(kJ \text{ mol}^{-1}) = 0.7 \]

(=7.9 to 9.3)
FIGURE 5.1.1.3.4 Logarithm of $K_{OW}$ versus reciprocal temperature for trichloromethane.
5.1.1.4 Tetrachloromethane (Carbon tetrachloride)

\[
\begin{array}{c}
\text{Cl} \\
\hline \\
\text{Cl} \\
\hline \\
\text{Cl} \\
\hline \\
\text{Cl}
\end{array}
\]

Common Name: Carbon tetrachloride
Synonym: tetrachloromethane, methane tetrachloride, perchloromethane, benzinoform
Chemical Name: tetrachloromethane
CAS Registry No: 56-23-5
Molecular Formula: CCl₄
Molecular Weight: 153.823

Melting Point (°C):
-22.62 (Lide 2003)
Boiling Point (°C):
76.8 (Lide 2003)

Density (g/cm³ at 20°C):
- 1.594 (McGovern 1943; Dreisbach 1959, 1961; Weast 1982–83; Horvath 1982; Riddick et al. 1986)
- 1.6037, 1.59402, 1.58436 (15, 20, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
- 113.2 (calculated-Le Bas method at normal boiling point)
- 96.0 (calculated-density, Wang et al. 1992)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
- 32.41, 29.96 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta H_{ fus } \) (kJ/mol):
- 0.775 (calculated, Dreisbach 1959)
- 0.581 (quoted, Riddick et al. 1986)

Entropy of Fusion, \( \Delta S_{ fus } \) (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 800, 850 (20°C, 30°C, volumetric method, Rex 1906)
- 770 (shake flask-interferometer, Gross 1929a,b)
- 770, 810 (15, 30°C, shake flask-interferometer, Gross & Saylor 1931)
- 780 (Seidell 1941)
- 800 (data presented in graph, temp range 0–70°C, McGovern 1943; Dilling 1977)
- 770 (15°C, Jones et al. 1957)
- 785 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
- 778 (20°C, recommended, Sørensen & Arit 1979)
- 800* (measured range 20–30°C, Andelman 1978)
- 757 (shake flask-LSC, Banerjee et al. 1980)
- 700 (shake flask-titration/turbidity, Coca et al. 1980)
- 793.4* (summary of literature data, Horvath 1982)
- 831 (calculated-UNIFAC activity coeff., Arbuckle 1983)
- 753 (calculated-UNIFAC activity coeff., Banerjee 1985)
- 800 (shake flask-radiometric method, Lo et al. 1986)
- 770 (selected, Riddick et al. 1986)
- 780 (23–24°C, shake flask-GC, Broholm et al. 1992)
- 600*, 720 (20.5, 31.0°C, shake flask-GC/TC, measured range 0–75°C, Stephenson 1992)
- 930, 873, 950, 982 (20, 30, 35, 40°C, infinite dilution activity coeff, \( \gamma^\prime \)-GC, Tse et al. 1992)
- 756, 896, 972, 1052 (20, 30, 35, 40°C, infinite dilution activity coeff, \( \gamma^\prime \)-UNIFAC, Tse et al. 1992)
- 700, 652, 652 (20, 30, 40°C, activity coeff, \( \gamma^\prime \)-differential pressure transducer, Wright et al. 1992)
- 701, 702 (20°C, calculated-activity coefficients, Wright et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17170, 18810 (20°C, 30°C, Rex 1906)
11372* (19.8°C, manometry, measured range 19.8–76.4°C, Smyth & Engel 1929)
15200 (extrapolated-Antoine eq., vapor-liquid equilibrium VLE data, measured range 30–70°C, Scatchard et al. 1939; quoted, Bissell & Williamson 1975)
log (P/mmHg) = 6.68148 – 1045.022/(T/K) – 99.577/(T/K)^2; temp range 30–70°C (VLE data, Scatchard et al. 1939)

15372* (25.2°C, temp range 14.06–76.84°C, Boublik 1960; quoted, Boublik et al. 1984)
log (P/mmHg) = 6.94369 – 1221.1/(224.0 + t°C); temp range –1 to 113°C (Antoine eq. for liquid state, Dreisbach 1961)
15220* (twin ebulliometer, measured range 20–77°C, Hildenbrand & McDonald 1959)
15230 (Marsh 1968; quoted, Bissell & Williamson 1975)
13200 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7628.8/(T/K)] + 7.586045; temp range –50 to 276°C (Antoine eq., Weast 1972–73)
15250, 15240 (calculated-Antoine eq., Boublik et al. 1973)

15170 (Daubert & Danner 1985)
log (P/mmHg) = 6.87926 – 1212.021/(226.409 + t°C); temp range 14.06–76.04°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1973)

15320 (selected summary of literature data, temp range 250.33–398.15 K, Xiang 2002)
18826 (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)
Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2912  (calculated as 1/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)
152.8 (calculated-bond method, Hine & Mookerjee 1975)
2216  (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
2776  (gas stripping-GC, Mackay et al. 1979)
2350  (20°C, calculated-P/C, Kavanaugh & Trussell 1980, 1983)
log (H/atm) = 10.06 – 2038.25/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)
2797* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
ln (kH/atm) = 22.22 – 4438/(T/K); temp range 1.0–27.2°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
2160  (calculated-P/C, Mackay & Shiu 1981)
2330  (20°C, calculated-P/C, Mabey et al. 1982)
2454  (20°C, batch stripping, Munz & Roberts 1982)
2418  (20°C, calculated-UNIFAC activity coeff., Arbuckle 1983)
3081  (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
ln K_{AW} = 9.77 – 2918/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.64  (Leo et al. 1971)
2.62  (shake flask-GC, Chiou et al. 1977)
2.83  (shake flask, Hansch & Leo 1979, 1987)
<table>
<thead>
<tr>
<th>Octanol/Air Partition Coefficient, log ( K_{OA} ) at 25°C:</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.73 (shake flask-LSC, Banerjee et al. 1980)</td>
</tr>
<tr>
<td>2.73 (shake flask-LSC, Veith et al. 1980)</td>
</tr>
<tr>
<td>2.94 (HPLC-( K^\prime ) correlation, McDuffie 1981)</td>
</tr>
<tr>
<td>2.81, 290 (calculated from UNIFAC activity coeff. with octanol and water mutual solubility considered, not considered, Arbuckle 1983)</td>
</tr>
<tr>
<td>2.83 (HPLC-( K^\prime ) correlation, Hafkenscheid &amp; Tomlinson 1983)</td>
</tr>
<tr>
<td>2.03 (HPLC correlation, Eadsforth 1986)</td>
</tr>
<tr>
<td>2.73 (HPLC-( K^\prime ) correlation, Tomlinson &amp; Hafkenscheid 1986)</td>
</tr>
<tr>
<td>2.38 (calculated-UNIFAC activity coefficients, Banerjee &amp; Howard 1988)</td>
</tr>
<tr>
<td>2.83 (recommended, Sangster 1989)</td>
</tr>
<tr>
<td>2.83 (recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>2.73* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia &amp; Sandler 1995)</td>
</tr>
<tr>
<td>2.38* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C:

2.79 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

1.24 (rainbow trout, Neely et al. 1974; Veith et al. 1979)

1.25 (trout muscle, calculated-ratio of rate const. \( k_1/k_2 \), Neely et al. 1974)

1.48 (bluegill sunfish, Barrows et al. 1980; Veith et al. 1980; Veith & Kosian 1982)

2.32 (microorganisms-water, calculated-\( K_{OW} \), Mabey et al. 1982)

1.72 (rainbow trout, Veith & Kosian 1982)

2.68 (activated sludge, Freitag et al. 1984)

2.48 (algae chlorella fusca-LSC, Geyer et al. 1984)

2.68, 2.48, < 1.0 (activated sludge, Chlorella fusca, golden ide, Freitag et al. 1985)

2.06 (calculated-\( K_{OW} \), \( S_{OCTANO} \) and mp, Banerjee & Baughman 1991)

Sorption Partition Coefficient, log \( K_{OC} \) at 25°C or as indicated:

2.04 (calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

2.64 (calculated-\( K_{MP} \), Mabey et al. 1982)

1.85 (calculated-MCI \( \chi \), Koch 1983)

1.70 (calculated-MCI \( \chi \), Bahnick & Doucette 1988)

2.26, 1.34, 1.70, 1.96, 2.07 (DTMA-clay, TTMA-clay, HTMA-clay, BDHA-clay, DDPA-clay, Smith et al. 1990)

1.69 (80% DTMA-clay at 20°C, Smith & Jaffé 1991)

2.16; 1.70; 2.06 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

2.20, 2.24, 2.24, 2.25, 2.28, 2.27, 2.33 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon \( f_{OC} = 4.12\% \), EPICS-GC/FID, Dewulf et al. 1999)

1.80, 1.80, 1.78 (soils: organic carbon OC \( \geq 0.1\% \), OC \( \geq 0.5\% \), 0.1 \( \leq \) OC < 0.5%, average, Delle Site 2001)

2.01, 2.00, 2.02 (sediments: organic carbon OC \( \geq 0.1\% \), OC \( \geq 0.5\% \), 0.1 \( \leq \) OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log \( K_{OM} \):

1.55 (calculated-MCI \( \chi \), Sabljic 1984)

1.89, 1.72 (Florida peat, OC 57.1%; Michigan muck, OC 53.1%, batch equilibrium-sorption equilibrium, Rutherford & Chiou 1992; Rutherford et al. 1992)

0.243, 1.866 (cellulose, extracted peat, Rutherford et al. 1992)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization: \( t_{1/2} = 29 \) min was determined in an open container with initial concentration of 1 mg/L when stirred at 100 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Verschueren 1983); Evaporation \( t_{1/2}(\text{exptl}) = 28.8 \) min, \( t_{1/2}(\text{calc}) = 0.2 \) min, 25.5 min from water (Dilling 1977);
ratio of evaporation rate constant to that of oxygen reaeration: 0.47 as measured value compared to 0.43 as predicted (Smith et al. 1980);
k < 2.4 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \text{ estimated rate constant for the reaction with OH radical at 300 K (Lyman 1982)};
t_{1/2} \sim 37 \text{ h from a model river of 1 m deep for water flowing at 1 m/s with wind speed of 3 m/s and Henry’s law constant (Thomas 1982; Lyman et al. 1982; quoted, Howard 1990).}

Photolysis: photocatalyzed mineralization by the presence of TiO$_2$ with the rate of 0.18 ppm/min per gram of catalyst (Ollis 1985).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH} < 1.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Cox et al. 1976)
- $k_{OH} = 1 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$ bimolecular reaction rate, with a reported tropospheric lifetime of greater than 330 yr (Cox et al. 1976; quoted, Callahan et al. 1979)
- $k_{OH} < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (discharge flow-LMR, Howard & Evenson 1976a)
- $k_{OH} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time > 11600 d, loss = 0.0% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
- $k_{OH}(calc) << 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k << 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
- $k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
- photooxidation half-life in air: $1.6 \times 10^4 - 1.6 \times 10^5$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: hydrolysis rate constant $k = 4.8 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 7000 \text{ yr (1 ppm)}$, $t_{1/2} = 7 \text{ yr (1000 ppm)}$ at 25°C and pH 7 (Mabey & Mill 1978)

calculated first-order $t_{1/2} = 7000 \text{ yr},$ based on reported rate constant $k = 4.8 \times 10^{-7} \text{ mol}^{-1} \text{ s}^{-1}$ for 1 mg/L concentration at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard 1990; Howard et al. 1991)

- $t_{1/2} = 2,600,000 \text{ d at pH 7 in natural waters (Capel & Larson 1995)}$

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 4320–8640 \text{ h},$ based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

- $t_{1/2}(\text{aq. anaerobic}) = 168–672 \text{ h},$ based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991) and acclimated anaerobic sediment/aquifer grab sample data (Parsons et al. 1985; quoted, Howard et al. 1991).

- $t_{1/2}(\text{aerobic}) = 170 \text{ d},$ $t_{1/2}(\text{anaerobic}) = 7 \text{ d in natural waters (Capel & Larson 1995)}$

Bioconcentration: estimated rate constant of $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria in water (Mabey et al. 1982).

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1 = 4.05 \text{ h}^{-1};$ $k_2 = 0.229 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974; quoted, Thomann 1989)
- $k_1 = 4.05 \text{ mL g}^{-1} \text{ h}^{-1}$ (10°C, trout gill, Neely 1979)
- $k_1 = 4.10 \text{ h}^{-1};$ $k_2 = 0.25 \text{ h}^{-1}$ (trout, Hawker & Connell 1985)

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 10 \text{ wk},$ when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

- disappearance $t_{1/2} > 10 \text{ d for the reaction with OH radical in air (Darnall et al. 1976);}$
- estimated residence time in troposphere, > 330 yr (CEQ 1975);
- estimated residence time of 100 yr in troposphere (Singh et al. 1979);
- residence time > 11600 d, loss = 0.0% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)
- estimated residence time of 4–20 yr in troposphere (Lyman 1982);
- $t_{1/2} = 30–50 \text{ yr residence time in the troposphere (Howard 1990);}$
- $t_{1/2} = 1.6 \times 10^4 - 1.6 \times 10^5 \text{ h, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).}$

Surface water: estimated $t_{1/2} = 0.4–56 \text{ d in various locations in the Netherlands in case of a first order reduction process; } t_{1/2} \sim 3–30 \text{ d in rivers and } t_{1/2} = 3–300 \text{ d in lakes (Zoeteman et al. 1980);}$

- $t_{1/2} = 4320–8640 \text{ h, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).}$

- $t_{1/2}(\text{aerobic}) = 170 \text{ d},$ $t_{1/2}(\text{anaerobic}) = 7 \text{ d in natural waters (Capel & Larson 1995)}$
Ground water: estimated $t_{1/2} \sim 3–300$ d (Zoeteman et al. 1980; quoted, Howard 1990); $t_{1/2} = 168–8640$ h, based on estimated aqueous aerobic biodegradation half-life and acclimated anaerobic sediment/aquifer grab sample data (Howard et al. 1991).

Sediment:
Soil: $t_{1/2} = 4320–8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
$\; t_{1/2}^{(calc)} = 50$ d in soil mixtures from first-order kinetic (Anderson et al. 1991).
Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980).

<table>
<thead>
<tr>
<th>TABLE 5.1.1.4.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities of tetrachloromethane at various temperatures</td>
</tr>
</tbody>
</table>

\[
S/(\text{wt}%) = 9.7842 \times 10^{-2} - 1.4942 \times 10^{-3} \cdot (t/°C) + 3.5854 \times 10^{-5} \cdot (t/°C)^2 + 2.2775 \times 10^{-7} \cdot (t/°C)^3 \quad (1)
\]

### 1.

<table>
<thead>
<tr>
<th>Rex 1906</th>
<th>Gross &amp; Saylor 1931</th>
<th>Andelman 1978</th>
<th>Horvath 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td>volumetric method</td>
<td>shake flask-IR</td>
<td>summary of literature data</td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
</tr>
<tr>
<td>20</td>
<td>800</td>
<td>15</td>
<td>770</td>
</tr>
<tr>
<td>30</td>
<td>850</td>
<td>30</td>
<td>810</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 2.

<table>
<thead>
<tr>
<th>Stephenson 1992</th>
<th>Tse et al. 1992</th>
<th>Wright et al. 1992</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC</td>
<td>activity coefficient</td>
<td>activity coefficient</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>0</td>
<td>890</td>
<td>20</td>
</tr>
<tr>
<td>10</td>
<td>630</td>
<td>30</td>
</tr>
<tr>
<td>20.5</td>
<td>600</td>
<td>35</td>
</tr>
<tr>
<td>31.0</td>
<td>720</td>
<td>40</td>
</tr>
<tr>
<td>41.3</td>
<td>680</td>
<td></td>
</tr>
<tr>
<td>52.5</td>
<td>780</td>
<td></td>
</tr>
<tr>
<td>64.0</td>
<td>960</td>
<td></td>
</tr>
<tr>
<td>75.0</td>
<td>1150</td>
<td></td>
</tr>
</tbody>
</table>
**FIGURE 5.1.1.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for tetrachloromethane.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
</tr>
<tr>
<td>19.2</td>
<td>11732</td>
<td>-50.0</td>
<td>133.3</td>
</tr>
<tr>
<td>32.4</td>
<td>20798</td>
<td>-30.0</td>
<td>666.6</td>
</tr>
<tr>
<td>41.2</td>
<td>29704</td>
<td>-19.6</td>
<td>1333</td>
</tr>
<tr>
<td>50.0</td>
<td>41597</td>
<td>-8.20</td>
<td>2666</td>
</tr>
<tr>
<td>60.8</td>
<td>60368</td>
<td>4.30</td>
<td>5333</td>
</tr>
<tr>
<td>68.7</td>
<td>78180</td>
<td>12.3</td>
<td>7999</td>
</tr>
<tr>
<td>76.4</td>
<td>101325</td>
<td>23.0</td>
<td>13332</td>
</tr>
<tr>
<td>bp/°C</td>
<td>76.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>76.7</td>
<td>101325</td>
<td>38.3</td>
<td>26664</td>
</tr>
<tr>
<td>bp/°C</td>
<td>76.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>-22.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Reported vapor pressures of tetrachloromethane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - B/(T/K) \\
\log P = A - B/(C + t/°C) \\
\log P = A - B/(C + T/K) \\
\log P = A - B/(T/K) - C \log (T/K)
\]

| static-manometer | summary of literature data | twin ebulliometer system | |
| **A** | 6.89406 | 6.00535 | 6.00535 |
| **B** | 1219.58 | 6.89406 | 1219.58 |
| **C** | 227.16 | | 227.16 |
| **bp/°C** | 76.714 | | 76.714 |

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
FIGURE 5.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.3
Reported Henry's law constants of tetrachloromethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{T/K} \quad (1) \\
\ln \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/K} \quad (2) \\
\ln H = A - \frac{B}{T/K} \quad (3) \\
K_{AW} = A - B \cdot \frac{T}{K} + C \cdot \left(\frac{T}{K}\right)^2 \quad (5)
\]

1. Leighton & Calo 1981

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>751.6</td>
<td>10.0</td>
<td>1337.5</td>
<td>10</td>
<td>1500</td>
<td>25</td>
<td>2875</td>
</tr>
<tr>
<td>1.3</td>
<td>752.2</td>
<td>17.5</td>
<td>2138</td>
<td>15</td>
<td>1935</td>
<td>26.5</td>
<td>2666</td>
</tr>
<tr>
<td>11.0</td>
<td>1312</td>
<td>24.8</td>
<td>3080</td>
<td>20</td>
<td>2351</td>
<td>27.4</td>
<td>3248</td>
</tr>
<tr>
<td>13.0</td>
<td>1568</td>
<td>34.6</td>
<td>4661</td>
<td>25</td>
<td>2989</td>
<td>28.9</td>
<td>3315</td>
</tr>
<tr>
<td>21.0</td>
<td>2335</td>
<td>30</td>
<td>3830</td>
<td>30</td>
<td>4713</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>22.0</td>
<td>2406</td>
<td>A</td>
<td>11.29</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>29.7</td>
<td>3525</td>
</tr>
<tr>
<td>27.1</td>
<td>2866</td>
<td>B</td>
<td>4411</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>25</td>
<td>2797</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2. Gossett 1987

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>751.6</td>
<td>10.0</td>
<td>1337.5</td>
<td>10</td>
<td>1500</td>
<td>25</td>
<td>2875</td>
</tr>
<tr>
<td>1.3</td>
<td>752.2</td>
<td>17.5</td>
<td>2138</td>
<td>15</td>
<td>1935</td>
<td>26.5</td>
<td>2666</td>
</tr>
<tr>
<td>11.0</td>
<td>1312</td>
<td>24.8</td>
<td>3080</td>
<td>20</td>
<td>2351</td>
<td>27.4</td>
<td>3248</td>
</tr>
<tr>
<td>13.0</td>
<td>1568</td>
<td>34.6</td>
<td>4661</td>
<td>25</td>
<td>2989</td>
<td>28.9</td>
<td>3315</td>
</tr>
<tr>
<td>21.0</td>
<td>2335</td>
<td>30</td>
<td>3830</td>
<td>30</td>
<td>4713</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>22.0</td>
<td>2406</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>29.7</td>
<td>3525</td>
</tr>
<tr>
<td>27.1</td>
<td>2866</td>
<td>A</td>
<td>11.29</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>25</td>
<td>2797</td>
<td>B</td>
<td>4411</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
</tbody>
</table>

3. Ashworth et al. 1988

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>751.6</td>
<td>10.0</td>
<td>1337.5</td>
<td>10</td>
<td>1500</td>
<td>25</td>
<td>2875</td>
</tr>
<tr>
<td>1.3</td>
<td>752.2</td>
<td>17.5</td>
<td>2138</td>
<td>15</td>
<td>1935</td>
<td>26.5</td>
<td>2666</td>
</tr>
<tr>
<td>11.0</td>
<td>1312</td>
<td>24.8</td>
<td>3080</td>
<td>20</td>
<td>2351</td>
<td>27.4</td>
<td>3248</td>
</tr>
<tr>
<td>13.0</td>
<td>1568</td>
<td>34.6</td>
<td>4661</td>
<td>25</td>
<td>2989</td>
<td>28.9</td>
<td>3315</td>
</tr>
<tr>
<td>21.0</td>
<td>2335</td>
<td>30</td>
<td>3830</td>
<td>30</td>
<td>4713</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>22.0</td>
<td>2406</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>29.7</td>
<td>3525</td>
</tr>
<tr>
<td>27.1</td>
<td>2866</td>
<td>A</td>
<td>11.29</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>25</td>
<td>2797</td>
<td>B</td>
<td>4411</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
</tbody>
</table>

4. Tancrédé & Yanagisawa 90

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>751.6</td>
<td>10.0</td>
<td>1337.5</td>
<td>10</td>
<td>1500</td>
<td>25</td>
<td>2875</td>
</tr>
<tr>
<td>1.3</td>
<td>752.2</td>
<td>17.5</td>
<td>2138</td>
<td>15</td>
<td>1935</td>
<td>26.5</td>
<td>2666</td>
</tr>
<tr>
<td>11.0</td>
<td>1312</td>
<td>24.8</td>
<td>3080</td>
<td>20</td>
<td>2351</td>
<td>27.4</td>
<td>3248</td>
</tr>
<tr>
<td>13.0</td>
<td>1568</td>
<td>34.6</td>
<td>4661</td>
<td>25</td>
<td>2989</td>
<td>28.9</td>
<td>3315</td>
</tr>
<tr>
<td>21.0</td>
<td>2335</td>
<td>30</td>
<td>3830</td>
<td>30</td>
<td>4713</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>22.0</td>
<td>2406</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>29.7</td>
<td>3525</td>
</tr>
<tr>
<td>27.1</td>
<td>2866</td>
<td>A</td>
<td>11.29</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
<tr>
<td>25</td>
<td>2797</td>
<td>B</td>
<td>4411</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>33.3</td>
<td>4713</td>
</tr>
</tbody>
</table>

(Continued)

<table>
<thead>
<tr>
<th>activity coefficient</th>
<th>activity coefficient</th>
<th>EPICS-GC</th>
<th>EPICS-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>20</td>
<td>2067</td>
<td>20</td>
<td>2646</td>
</tr>
<tr>
<td>30</td>
<td>3415</td>
<td>35</td>
<td>4550</td>
</tr>
<tr>
<td>35</td>
<td>3871</td>
<td>50</td>
<td>6624</td>
</tr>
<tr>
<td>40</td>
<td>4580</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.4.3 Logarithm of Henry’s law constant versus reciprocal temperature for tetrachloromethane.
TABLE 5.1.1.4.4
Reported octanol-water partition coefficients of tetrachloromethane at various temperatures

<table>
<thead>
<tr>
<th>Relative GC-RT technique</th>
<th>EPICS-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>log K_{OW}</td>
</tr>
<tr>
<td>25</td>
<td>2.73</td>
</tr>
<tr>
<td>35</td>
<td>2.74</td>
</tr>
<tr>
<td>50</td>
<td>2.73</td>
</tr>
<tr>
<td>14.1</td>
<td>2.44</td>
</tr>
<tr>
<td>18.7</td>
<td>2.47</td>
</tr>
</tbody>
</table>

Change in enthalpy:
\[ \Delta H_{OW}/(kJ \text{ mol}^{-1}) = 1.3 \]
\((-12.1 \text{ to } 14.6)\)

Enthalpy of transfer:
\[ \Delta H_{oct}/(kJ \text{ mol}^{-1}) = -0.5 \]
\((-13.9 \text{ to } 12.8)\)

FIGURE 5.1.1.4.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloromethane.
5.1.1.5 Chloroethane (Ethyl chloride)

[Chemical structure diagram]

Common Name: Ethyl chloride
Synonym: chloroethane, monochloroethane
Chemical Name: chloroethane, ethyl chloride, monochloroethane, hydrochloric ether, muriatic ether
CAS Registry No: 75-00-3
Molecular Formula: C₂H₅Cl, CH₃CH₂Cl
Molecular Weight: 64.514
Melting Point (°C):
-138.4 (Lide 2003)
Boiling Point (°C):
12.30 (McGovern 1943; Weast 1982–83; Dean 1985; Howard 1990; Lide 2003)
Density (g/cm³ at 20°C):
0.8978 (Weast 1982–83)
0.92390, 0.8960, 0.88981 (0, 20, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
72.0 (calculated-density, Wang et al. 1992)
72.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
27.8, 24.652 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHₚ (kJ/mol):
4.45 (Riddick et al. 1986)
Entropy of Fusion, ΔSₚ (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
5735 (12.5°C, shake flask, Fühner 1924)
7580 (Seidell 1940)
4500 (0°C, McGovern 1943; Dean 1985)
5710 (20°C, Neely 1976)
5700 (20°C, selected, Dilling 1977)
5678* (20°C, summary of literature data, Horvath 1982)
5740 (20°C, Verschueren 1977, 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
136630 (data presented in graph, temp range ~50 to ~105°C, McGovern 1943)
187000* (extrapolated-Antoine eq. regression, summary of literature data, Stull 1947)
101436* (12.51°C, static method-Hg manometer, measured range ~55.88 to 12.51°C, Gordon & Giauque 1948)
160000 (calculated-Antoine eq., Dreisbach 1959)

\[
\log (P/\text{mmHg}) = 6.94914 - \frac{1012.771}{(236.47 + t/^\circ \text{C})}; \text{ temp range } \sim 50 \text{ to } 70^\circ \text{C} \text{ (Antoine eq. for liquid state, Dreisbach 1959)}
\]
\[
\log (P/\text{mmHg}) = 6.94914 - \frac{1012.771}{(236.67 + t/^\circ \text{C})}, \text{ pressure range of 10 to 1500 mmHg, (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)}
\]
\[
\log (P/\text{mmHg}) = [-0.2185 \times 6310.6/(T/K)] + 7.660205; \text{ temp range } \sim 89.8 \text{ to } 180.5^\circ \text{C} \text{ (Antoine eq., Weast 1972–73)}
\]
160000 (calculated-Antoine eq., Boublík et al. 1973)
\[
\log (P/\text{mmHg}) = 6.98647 - \frac{1030.007}{(236.612 + t/^\circ \text{C})}; \text{ temp range } \sim 55.94 \text{ to } 12.5^\circ \text{C} \text{ (Antoine eq. from reported exptl. data, Boublík et al. 1973)}
\]
149400 (extrapolated-Antoine eq., Boublík et al. 1984)
\[
\log (P/\text{kPa}) = 6.11833 - \frac{1033.161}{(236.956 + t/^\circ \text{C})}; \text{ temp range } \sim 55.94 \text{ to } 12.5^\circ \text{C} \text{ (Antoine eq. from reported exptl. data, Boublík et al. 1984)}
\]
log (P/mmHg) = 6.98647 – 1030.01/(238.61 + t/°C); temp range −56 to 12.2°C (Antoine eq., Dean 1985, 1992)

159880 (selected, Riddick et al. 1986)

log (P/kPa) = 6.09088 – 1020.63/(237.57 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

160000 (calculated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.07404 – 1012.771/(–36.48 + T/K); temp range 207–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.14258 – 1053.998/(–30.68 + T/K); temp range 285–460 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.4495 – 1248.788/(–3.79 + T/K); temp range: 334–413 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.70739 – 1465.734/(29.69 + T/K); temp range 403–460 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 28.3448 – 2.0788 × 103/(T/K) – 7.5387·log (T/K) – 1.6384 × 10–11·(T/K)+4.055×10–6·(T/K)2; temp range 137–460 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

860 (calculated as 1/K AW, Cq/C A, reported as exp., Hine & Mookerjee 1975)

1140 (calculated, Dilling 1977)


1125* (24.8°C, EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)

ln [H/(atm m³/mol)] = 5.974 – 3120/(T/K); temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)

1226* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm-m³/mol)] = 4.265 – 2580/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

1270 (calculated-QSAR, Nirmalakhandan & Speece 1988)

942 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

701 (computed value, Yaws et al. 1991)

1019 (20°C, selected from reported experimental determined values, Staedinger & Roberts 1996, 2001)

log K AW = 3.406 – 1110/(T/K) (summary of literature data, Staedinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K OW:

1.54 (Leo et al. 1971)

1.39 (calculated-π substituent const., Hansch et al. 1968; Hansch & Leo 1979)

1.43 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1987)

1.43 (recommended, Sangster 1989, 1993)

1.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K OA:

Belconcentration Factor, log BCF:

0.86, 0.67 (estimated-K OW, S, Lyman et al. 1982; quoted, Howard et al. 1990)

0.99 (microorganisms-water, calculated-K OW, Mabey et al. 1982)

Sorption Partition Coefficient, log K OC:

2.16, 1.52 (estimated-K OW, S, Lyman et al. 1982; quoted, Howard 1990)

1.17 (sediment-water, calculated-K OW, Mabey et al. 1982)

1.40 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, k, and Half-Lives, t½:

V olatilization: estimated experimental t½ = 21 min for 1 mg/L to evaporate from aqueous solution stirred at 200 rpm in an open container of depth 65 mm at 25°C (Dilling et al. 1975);

Evaporation t½(exptl) = 23.1 min, t½(calc) = 0.5 min, 16.7 min from water (Dilling 1977);

volatilization t½ = 2.5 h from a model river of 1 m deep, based on Henry’s law constant (Lyman et al. 1982; quoted, Howard 1990);
Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3, or as indicated, *data at other temperatures and/or the Arrhenius expression

\[
k_{OH} = (3.9 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K}
\]

and the calculated lifetime of about \( 2.6 \times 10^8 \text{ s} \) or 30 d (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980)

\[
k_{OH} = (3.9 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K}
\]

or (3.94 \pm 0.53) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 297 \text{ K} (flash photolysis-resonance fluorescence, Paraskievopoulos et al. 1978)

\[
k_{OH} = 2.3 \times 10^{13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K} \text{ (Lyman 1982)}
\]

\[
k < 360 \text{ M}^{-1} \text{ h}^{-1} \text{ for singlet oxygen and } k < 1 \text{ M}^{-1} \text{ h}^{-1} \text{ for peroxy radical (Mabey et al. 1982)}
\]

\[
k_{O3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{, measured range } 298–323 \text{ K} \text{ (quoted, Atkinson & Carter 1984)}
\]

Photooxidation half-life of 160–1604 h, based on measured rate constants for the reaction with OH radical in air (Atkinson 1985; quoted, Howard 1990; Howard et al. 1991)

\[
k_{OH} = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (recommended, Atkinson 1989)}
\]

\[
k_{OH} = (4.08 \pm 0.31) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294.8 \text{ K} \text{, measured range } 294.8–788.7 \text{ K (laser photolysis/laser induced fluorescence, Kasner et al. 1990)}
\]

Hydrolysis: \( k = 2.0 \times 10^{-7} \text{ s}^{-1} \) was estimated for reaction at pH 7 and 25°C with a maximum \( t_{1/2} = 40 \text{ d} \) (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

\[
k = 2.10 \times 10^{-7} \text{ s}^{-1} \text{ with } t_{1/2} = 38 \text{ day at } 25^\circ \text{C and pH 7} \text{ (Mabey & Mill 1978)}
\]

estimated \( t_{1/2} = 38 \text{ d} \text{ at } 25^\circ \text{C} \text{ was based on an exptl } t_{1/2} = 1.68 \text{ h} \text{ at } 100^\circ \text{C with ethanol and HCl being the hydrolysis product (Mabey & Mill 1978; quoted, Haque et al. 1980; Howard 1990; Howard et al. 1991);}

\[
k = 4.5 \times 10^{-3} \text{ s}^{-1} \text{ at } 25^\circ \text{C and pH 7} \text{ with a calculated } t_{1/2} = 1.8 \text{ yr} \text{ (Jeffers et al. 1989; quoted, Ellington 1989);}
\]

Abiotic hydrolysis or dehydrohalogenation \( t_{1/2} = 1.3 \text{ month} \text{ (Olsen & Davis 1990)}. \)

Biodegradation:

\[
t_{1/2}(\text{aq. aerobic}) = 168–672 \text{ h}, \text{ based on aqueous aerobic screening test data for 1-chloropropane and 1-chlorobutane (Gerhold & Malaney 1966; quoted, Howard et al. 1991)}
\]

\[
t_{1/2}(\text{anaerobic}) = 672–2688 \text{ h}, \text{ based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991)}
\]

\[
k = 0.02 \text{ yr}^{-1} \text{ with } t_{1/2} = 10 \text{ d} \text{ and } k = 0.001 \text{ yr}^{-1} \text{ with } t_{1/2} = 700 \text{ d} \text{ (Olsen & Davis 1990).}
\]

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance \( t_{1/2} = 2.4–24 \text{ h} \text{ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);}

\[
\text{calculated lifetime of about } 2.6 \times 10^8 \text{ s} \text{ or } 30 \text{ d} \text{ (Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980);}
\]

\[
t_{1/2} = 160–1604 \text{ h}, \text{ based on photooxidation half-life in air from measured rate constants for the gas phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);}
\]

\[
\text{estimated tropospheric lifetime of } 0.04 \text{ yr} \text{ (Nimitz & Skaggs 1992).}\n\]

Surface water: \( t_{1/2} = 168–672 \text{ h}, \text{ based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).}
\]

Ground water: \( t_{1/2} = 336–1344 \text{ h}, \text{ based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).}
\]

Sediment:

\[
t_{1/2} = 10–50 \text{ d} \text{ (Ryan et al. 1988);}
\]

\[
t_{1/2} = 30 \text{ d}, \text{ volatilization loss from soil (Jury et al. 1990);}
\]

\[
t_{1/2} = 168–672 \text{ h}, \text{ based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).}
\]

Biota: \( t_{1/2} = 10–50 \text{ d}, \text{ subject to plant uptake by soil through volatilization (Ryan et al. 1988).} \)
TABLE 5.1.1.5.1
Reported aqueous solubilities and vapor pressures of chloroethane at various temperatures

\[
S/(\text{wt%}) = 0.5842 - 1.6863 \times 10^{-3} (t/°C) + 9.3949 \times 10^{-5} (t/°C)^2 - 2.5316 \times 10^{-6} (t/°C)^3
\]  (1)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility S/(g·m(^{-3}))</th>
<th>Vapor pressure P/(Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>58.42</td>
<td>133.3</td>
</tr>
<tr>
<td>10</td>
<td>57.42</td>
<td>666.6</td>
</tr>
<tr>
<td>20</td>
<td>56.78</td>
<td>1333</td>
</tr>
<tr>
<td>eq. 1</td>
<td>58.42</td>
<td>133.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility S/(g·m(^{-3}))</th>
<th>Vapor pressure P/(Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>58.42</td>
<td>133.3</td>
</tr>
<tr>
<td>10</td>
<td>57.42</td>
<td>666.6</td>
</tr>
<tr>
<td>20</td>
<td>56.78</td>
<td>1333</td>
</tr>
<tr>
<td>eq. 1</td>
<td>58.42</td>
<td>133.3</td>
</tr>
</tbody>
</table>

mp/°C = –139

mp/K = 134.80

bp/K = 285.37

log P = A – B/(T/K) – C·(T/K) + D·(T/K)^2

A = 10.54417
B = 1777.378
C = 0.0115789
D = 1.06734 \times 10^5

\[\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 4.452\]

\[\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 24.65\]

at 285.37 K

FIGURE 5.1.1.5.1 Logarithm of mole fraction solubility (ln \(x\)) versus reciprocal temperature for chloroethane.
**TABLE 5.1.1.5.2**
Reported Henry’s law constants of chloroethane at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \quad (1) \\
\ln (1/K_{AW}) &= A - B/(T/K) \quad (2) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \quad (3) \\
\ln \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] &= A - B/(T/K) \quad (4) \\
K_{AW} &= A - B(T/K) + C(T/K)^2 \quad (5)
\end{align*}
\]

Gossett 1987

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.3</td>
<td>660</td>
<td>10</td>
<td>769</td>
</tr>
<tr>
<td>17.5</td>
<td>857.2</td>
<td>15</td>
<td>970.7</td>
</tr>
<tr>
<td>24.8</td>
<td>1125</td>
<td>20</td>
<td>1115</td>
</tr>
<tr>
<td>34.6</td>
<td>1571</td>
<td>25</td>
<td>1226</td>
</tr>
<tr>
<td></td>
<td>eq. 4a</td>
<td>30</td>
<td>1449</td>
</tr>
<tr>
<td>A</td>
<td>7.385</td>
<td></td>
<td>eq. 4a</td>
</tr>
<tr>
<td>B</td>
<td>3286</td>
<td></td>
<td>A</td>
</tr>
</tbody>
</table>

Ashworth et al. 1988

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(atm m³/mol)</th>
<th>t/°C</th>
<th>H/(atm m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td></td>
<td>A</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td></td>
<td>B</td>
</tr>
<tr>
<td></td>
<td>4,265</td>
<td></td>
<td>2,580</td>
</tr>
</tbody>
</table>
FIGURE 5.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethane.
5.1.1.6 1,1-Dichloroethane

Common Name: 1,1-Dichloroethane
Synonym: ethylidene chloride, ethylidene dichloride
Chemical Name: 1,1-dichloroethane
CAS Registry No: 75-34-3
Molecular Formula: C₂H₄Cl₂, CH₃CHCl₂
Molecular Weight: 98.959
Melting Point (°C):
-96.9 (Lide 2003)
Boiling Point (°C):
57.3 (Weast 1982–83, Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.1757 (Dreisbach 1961; Horvath 1982; Weast 1982–83; Dean 1985)
1.1755, 1.1679 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
84.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
93.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
30.62, 28.6 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
7.87 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
5500* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
5060 (shake flask-interferometer, Gross 1929; quoted, Horvath 1982)
5555 (volumetric method, Wright & Schaffer 1932)
5060* (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
5060 (Seidell 1941)
4800* (shake flask, measured range 10–70°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 15.116 + 0.0230·(T/K), temp range 10–70°C, Walraevens et al. 1974
5100 (literature average, Dilling 1977, 1982)
4767* (summary of literature data, temp range 0–80°C, Horvath 1982)
4834 (30°C, headspace-GC analysis, McNally & Grob 1983)
4589 (30°C, headspace-GC analysis, McNally & Grob 1984)
5030 (20°C, selected, Riddick et al. 1986)
5090, 4910, 5090 (20, 35, 50°C, infinite dilution activity coeff. γ∞-GC, Barr & Newsham 1987)
4842, 4984 (predicted-MCI χ and polarizability, Nirmalakhadan & Speece 1988)
5240, 5317, 5406 (20, 30, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)
6560, 7300, 8085 (20, 30, 40°C, infinite dilution activity coeff. γ∞-UNIFAC, Tse et al. 1992)
4998, 4434, 5236 (20, 35, 45°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
5196* (20°C, activity coeff. by inert air stripping-GC, measured range 10–50°C, Hovorka & Dohnal 1997)
5040* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 9.4136 – 5.7249 × 10⁻²·(T/K) + 9.17839 × 10⁻⁵·(T/K)², temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
24300, 37000 (20°C, 30°C, Rex 1906)
30000* (Antoine eq. regression, temp range –60.7 to 57.4°C, Stull 1947)
22001* (17.62°C, static-Hg manometer, measured range –38.76 to 17.62°C, Li & Pitzer 1956)
30400 (calculated-Antoine eq., Dreisbach 1961)

\[ \log (P/\text{mmHg}) = \frac{6}{9853} - \frac{1171.42}{228.12 + t/\degree \text{C}}; \text{ temp range } –15 \text{ to } 82 \degree \text{C} \] (Antoine eq. for liquid state, Dreisbach 1961)

26000 (calculated-Antoine eq., Weast 1972–73)

\[ \log (P/\text{mmHg}) = [-0.2185 \times 7288.0/(T/\text{K})] + 7.629952; \text{ temp range } –60.7 \text{ to } 261.5 \degree \text{C} \] (Antoine eq., Weast 1972–73)

30260 (calculated-Antoine eq., Boublik et al. 1973)

\[ \log (P/\text{mmHg}) = \frac{6.97702 - 1174.022}{229.06 + t/\degree \text{C}}; \text{ temp range } –38.8 \text{ to } 17.6 \degree \text{C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1973)

30260 (Boublik et al. 1984)

\[ \log (P/\text{mmHg}) = \frac{6.10983 - 1177.636}{229.409 + t/\degree \text{C}}; \text{ temp range } –38.8 \text{ to } 17.5 \degree \text{C} \] (Antoine eq., Riddick et al. 1986)

30360 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log (P/L/\text{KPa}) = \frac{6.11002 - 1171.420}{T/\text{K} - 45.03} \] (from database of CDATA 1991, Hovorka & Dohnal 1997)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

595 (calculated-I/Kₐₐₕ (Cₜ /Cₐ) reported as exptl., Hine & Mookerjee 1975)
595 (calculated-P/C, Dilling 1977)

\[ \log (kₐ/atm) = 8.87 - 1902.37/(T/\text{K}) \] (least-square regression of data from lit., Kavanaugh & Trussell 1980)

633* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

\[ \ln [\text{H/(atm·m}^3/\text{mol})] = 5.484 - 3137/(T/\text{K}); \text{ temp range } 10–30 \degree \text{C} \] (EPICS measurements, Ashworth et al. 1988)

588, 1125, 1844 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

511* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)

24440, 37240 54990 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)

\[ \log (P/\text{mmHg}) = 33.380 - 2.6102 \times 10^3/(T/\text{K}) - 9.1336 \cdot \log (T/\text{K}) - 2.8838 \times 10^{-11} \cdot (T/\text{K})^2; \text{ temp range } 176–523 \degree \text{C} \] (vapor pressure eq., Yaws 1994)

588, 1125, 1844 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

511* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)


\[ \ln K_{ₐₐₙ} = -3975/(T/\text{K}) + 0.00768 \cdot Z + 11.727; \text{ with Z salinity 0–35.5‰, temp range: } 2–35 \degree \text{C} \] (EPICS-GC/FID, Dewulf et al. 1995)

466* (20°C, equilibrium air stripping-GC, measured range 10–50°C, Hovorka & Dohnal 1997)
500 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

\[ \log K_{ₐₐₙ} = 4.416 - 1498/(T/\text{K}) \] (summary of literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.79</td>
<td>(shake flask-GC, Hansch et al. 1975, Hansch &amp; Leo 1987)</td>
</tr>
<tr>
<td>1.92</td>
<td>(Hansch &amp; Leo 1979)</td>
</tr>
<tr>
<td>1.79</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>1.89</td>
<td>(calculated-activity coefficients, Tse &amp; Sandler 1994)</td>
</tr>
<tr>
<td>1.82*</td>
<td>(infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia &amp; Sandler 1995)</td>
</tr>
<tr>
<td>1.79</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>1.75*</td>
<td>(24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C:

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.41</td>
<td>(calculated-measured infinite dilution activity coeff. and vapor pressure $P$, Abraham et al. 2001)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.20</td>
<td>(estimated-S, Lyman et al. 1982)</td>
</tr>
<tr>
<td>1.28</td>
<td>(microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.60</td>
<td>(estimated-S, Lyman et al. 1982)</td>
</tr>
<tr>
<td>1.48</td>
<td>(sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>1.66</td>
<td>(soil, selected, Jury et al. 1990)</td>
</tr>
<tr>
<td>1.43, 1.46, 1.48, 1.50, 1.49, 1.55 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC}$ = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)</td>
<td></td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization: estimated experimental $t_\frac{1}{2} = 22$ min for initial concentration of 1.0 mg/L when stirred at 200 rpm in water at approx. 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_\frac{1}{2}(\text{exptl}) = 32.2$ min, $t_\frac{1}{2}(\text{calc}) = 0.98$ min, 21.2 min from water (Dilling 1977);

$t_\frac{1}{2} = 6–9$ d in a typical pond, $t_\frac{1}{2} = 5–8$ d in a typical lake, and $t_\frac{1}{2} = 24–32$ h in a typical river (Smith et al. 1980; quoted, Howard 1990);

ratio of rate of evaporation to that of oxygen reaeration: measured value of 0.57 compared to that predicted value of 0.47 (Smith et al. 1980);

$t_\frac{1}{2} = 45$ d for the volatilization loss from soil (Jury et al. 1990).

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO radical and $k_{O3}$ with O radicals or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.6 \pm 0.6) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980; Howard 1990)

$k_{OH} = 2.6 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 44 d, loss of 2.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{OH} < 1.6 \times 10^{17}$ cm$^3$ mol$^{-1}$ s$^{-1}$ for the reaction with OH radical at 300 K (Lyman 1982)

$k \ll 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and 1.0 M$^{-1}$ h$^{-1}$ for peroxy radical both at 25°C (Mabey et al. 1982; quoted, Ma et al. 1990)

Photooxidation $t_\frac{1}{2} = 247–2468$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: $k = 1.15 \times 10^{-7}$ M$^{-1}$ h$^{-1}$ for neutral process by analogy to dichloromethane (Mabey et al. 1982);

$k = 1.29 \times 10^{-6}$ h$^{-1}$ at pH 7 and 25°C with calculated $t_\frac{1}{2} = 61$ yr (Jeffers et al. 1989; quoted, Ellington 1989).

Biodegradation: $t_{50}(\text{aq. aerobic}) = 768–3696$ h, based on estimated methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a ground water aquifer
Halogenated Aliphatic Hydrocarbons

(Wilson et al. 1983; quoted, Howard et al. 1991); t½(aq. anaerobic) = 3072–14784 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

\[ t_{\text{aq. anaerobic}} > 60 \text{ d (Olsen \& Davis 1990).} \]

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance t½ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
calculated lifetime of 1.5 months based on reaction with OH radical (Callahan et al. 1979; Altschuller 1980; Howard 1990);
residence time of 44 d, loss of 2.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
\[ t_{\text{aq. anaerobic}} = 247–2468 \text{ h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);} \]
estimated tropospheric lifetime of 0.02 yr (Nimitz & Skaggs 1992).
Surface water: t½ = 768–3696 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: t½ = 10–50 d (Ryan et al. 1988);
\[ t_{\text{aq. anaerobic}} = 768–3696 \text{ h, based on methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991);} \]

Biotra: t½ = 45 d, volatilization loss from soil (Jury et al. 1990).

Biota: t½ < 2 d of elimination from whole body of bluegill sunfish (USEPA 1980; quoted, Howard 1990);
\[ t_{\text{aq. anaerobic}} = 10–50 \text{ d, subject to plant uptake via volatilization (Ryan et al. 1988).} \]

<table>
<thead>
<tr>
<th>TABLE 5.1.1.6.1</th>
</tr>
</thead>
</table>

Reported aqueous solubilities of 1,1-dichloroethane at various temperatures

\[ S/(\text{wt}\%) = 0.5826 - 7.8236 \times 10^{-3} \cdot (t/°C) + 1.5268 \times 10^{-4} \cdot (t/°C)^2 - 3.6609 \times 10^{-7} \cdot (t/°C)^3 \]  \[ (1) \]

\[ S/(\text{wt}\%) = 9.4136 - 5.7249 \times 10^{-2} \cdot (T/K) + 9.17839 \times 10^{-5} \cdot (T/K)^2 \]  \[ (2) \]

1.

<table>
<thead>
<tr>
<th>Rex 1906</th>
<th>Van Arkel &amp; Vles 1936</th>
<th>Walraevens et al. 1974</th>
<th>Horvath 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td>volumetric method</td>
<td>shake flask</td>
<td>shake flask-GC</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>0</td>
<td>6560</td>
<td>0</td>
<td>5940</td>
</tr>
<tr>
<td>10</td>
<td>5950</td>
<td>20</td>
<td>5060</td>
</tr>
<tr>
<td>20</td>
<td>5500</td>
<td>35</td>
<td>4820</td>
</tr>
<tr>
<td>30</td>
<td>5400</td>
<td>50</td>
<td>5190</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
### Table 5.1.1.6.1 (Continued)

<table>
<thead>
<tr>
<th>Source</th>
<th>infinite dilution activity coeff.</th>
<th>activity coefficient</th>
<th>activity coefficient</th>
<th>recommended, IUPAC-NIST</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>Barr &amp; Newsham 1987</td>
<td>20</td>
<td>5090</td>
<td>20</td>
<td>4998</td>
</tr>
<tr>
<td>Wright et al. 1992</td>
<td>35</td>
<td>4910</td>
<td>35</td>
<td>4434</td>
</tr>
<tr>
<td>Hovorka &amp; Dohnal 1997</td>
<td>50</td>
<td>5090</td>
<td>45</td>
<td>5236</td>
</tr>
<tr>
<td>Horvath &amp; Getzen 1999a</td>
<td>35</td>
<td>5266</td>
<td>15</td>
<td>5380</td>
</tr>
<tr>
<td>Tse et al. 1992</td>
<td>45</td>
<td>5576</td>
<td>25</td>
<td>5040</td>
</tr>
</tbody>
</table>

**Figure 5.1.1.6.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1-dichloroethane.
TABLE 5.1.1.6.2
Reported vapor pressures of 1,1-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>log P = A – B/(T/K)</th>
<th>ln P = A – B/(T/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>log P = A – B/(C + t°C)</td>
<td>ln P = A – B/(C + t°C)</td>
</tr>
<tr>
<td>log P = A – B/(C + T/K)</td>
<td></td>
</tr>
<tr>
<td>log P = A – B/(T/K) – C·log (T/K)</td>
<td></td>
</tr>
</tbody>
</table>

Stull 1947

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–60.7</td>
<td>133.3</td>
<td>–38.76</td>
<td>858.6</td>
<td>11.34</td>
<td>16536</td>
</tr>
<tr>
<td>–41.9</td>
<td>666.6</td>
<td>–29.61</td>
<td>1649</td>
<td>17.50</td>
<td>21876</td>
</tr>
<tr>
<td>–32.3</td>
<td>1333</td>
<td>–20.21</td>
<td>3020</td>
<td>17.62</td>
<td>22001</td>
</tr>
<tr>
<td>–21.9</td>
<td>2666</td>
<td>–19.18</td>
<td>3234</td>
<td></td>
<td></td>
</tr>
<tr>
<td>–10.2</td>
<td>5333</td>
<td>–18.16</td>
<td>3301</td>
<td>mp°C</td>
<td>–96.98</td>
</tr>
<tr>
<td>–2.90</td>
<td>7999</td>
<td>–17.69</td>
<td>3517</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.20</td>
<td>13332</td>
<td>–16.82</td>
<td>3716</td>
<td>eq. 2</td>
<td>P/cmHg</td>
</tr>
<tr>
<td>22.4</td>
<td>26664</td>
<td>–12.61</td>
<td>4772</td>
<td>A</td>
<td>6.1560</td>
</tr>
<tr>
<td>39.8</td>
<td>53329</td>
<td>–12.20</td>
<td>4869</td>
<td>B</td>
<td>1258.1</td>
</tr>
<tr>
<td>57.4</td>
<td>101325</td>
<td>–2.23</td>
<td>8425</td>
<td>C</td>
<td>26.0</td>
</tr>
<tr>
<td>mp°C</td>
<td>–96.7</td>
<td>1.18</td>
<td>10077</td>
<td>∆H_fus/(kJ mol⁻¹) = 7.87</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Li & Pitzer 1956

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–60.7</td>
<td>133.3</td>
<td>–38.76</td>
<td>858.6</td>
<td>11.34</td>
<td>16536</td>
</tr>
<tr>
<td>–41.9</td>
<td>666.6</td>
<td>–29.61</td>
<td>1649</td>
<td>17.50</td>
<td>21876</td>
</tr>
<tr>
<td>–32.3</td>
<td>1333</td>
<td>–20.21</td>
<td>3020</td>
<td>17.62</td>
<td>22001</td>
</tr>
<tr>
<td>–21.9</td>
<td>2666</td>
<td>–19.18</td>
<td>3234</td>
<td></td>
<td></td>
</tr>
<tr>
<td>–10.2</td>
<td>5333</td>
<td>–18.16</td>
<td>3301</td>
<td>mp°C</td>
<td>–96.98</td>
</tr>
<tr>
<td>–2.90</td>
<td>7999</td>
<td>–17.69</td>
<td>3517</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.20</td>
<td>13332</td>
<td>–16.82</td>
<td>3716</td>
<td>eq. 2</td>
<td>P/cmHg</td>
</tr>
<tr>
<td>22.4</td>
<td>26664</td>
<td>–12.61</td>
<td>4772</td>
<td>A</td>
<td>6.1560</td>
</tr>
<tr>
<td>39.8</td>
<td>53329</td>
<td>–12.20</td>
<td>4869</td>
<td>B</td>
<td>1258.1</td>
</tr>
<tr>
<td>57.4</td>
<td>101325</td>
<td>–2.23</td>
<td>8425</td>
<td>C</td>
<td>26.0</td>
</tr>
<tr>
<td>mp°C</td>
<td>–96.7</td>
<td>1.18</td>
<td>10077</td>
<td>∆H_fus/(kJ mol⁻¹) = 7.87</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethane.
TABLE 5.1.1.6.3
Reported Henry’s law constants of 1,1-dichloroethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{T/\text{K}} \quad (1)
\]
\[
\log K_{AW} = A - \frac{B}{T/\text{K}} \quad (1a)
\]
\[
\ln \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/\text{K}} \quad (2)
\]
\[
\log \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/\text{K}} \quad (2a)
\]
\[
\ln (k_H/\text{atm}) = A - \frac{B}{T/\text{K}} \quad (3)
\]
\[
\ln H = A - \frac{B}{T/\text{K}} \quad (4)
\]
\[
\log H = A - \frac{B}{T/\text{K}} \quad (4a)
\]
\[
K_{AW} = A - B \cdot \left(\frac{T}{\text{K}}\right) + C \cdot \left(\frac{T}{\text{K}}\right)^2 \quad (5)
\]

1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>EPICS-GC</strong></td>
<td><strong>EPICS-GC</strong></td>
<td>activity coefficient</td>
<td>activity coefficient</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
</tr>
<tr>
<td>9.6</td>
<td>251.3</td>
<td>10</td>
<td>373</td>
</tr>
<tr>
<td>17.5</td>
<td>394.2</td>
<td>15</td>
<td>460</td>
</tr>
<tr>
<td>24.8</td>
<td>569.4</td>
<td>20</td>
<td>570</td>
</tr>
<tr>
<td>34.6</td>
<td>820.7</td>
<td>25</td>
<td>631</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>786</td>
</tr>
<tr>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
</tr>
<tr>
<td>A</td>
<td>8.637</td>
<td>A</td>
<td>5.484</td>
</tr>
<tr>
<td>B</td>
<td>4128</td>
<td>B</td>
<td>3137</td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>activity coefficient</strong></td>
<td><strong>EPICS-GC</strong></td>
<td><strong>equilibrium air stripping-GC</strong></td>
<td><strong>EPICS-SPME method</strong></td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
</tr>
<tr>
<td>25</td>
<td>588</td>
<td>2</td>
<td>152.1</td>
</tr>
<tr>
<td>35</td>
<td>1125</td>
<td>6</td>
<td>195.2</td>
</tr>
<tr>
<td>50</td>
<td>1844</td>
<td>10</td>
<td>194.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>18.2</td>
<td>378.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>510.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1</td>
<td>K_{AW}</td>
<td>50</td>
<td>1338</td>
</tr>
<tr>
<td>A</td>
<td>11.727</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3975</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1</td>
<td>K_{AW}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>10.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3447.7</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.6.3 Logarithm of Henry’s law constant versus reciprocal temperature for 1,1-dichloroethane.

### TABLE 5.1.1.6.4
Reported octanol-water partition coefficients of 1,1-dichloroethane at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Bhatia &amp; Sandler 1995</th>
<th>DeWulf et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>log K&lt;sub&gt;OW&lt;/sub&gt;</td>
<td>EPICS-GC</td>
</tr>
<tr>
<td>25</td>
<td>1.82</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>1.66</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>1.68</td>
<td></td>
</tr>
<tr>
<td>2.2</td>
<td>1.70</td>
<td></td>
</tr>
<tr>
<td>4.0</td>
<td>1.69</td>
<td></td>
</tr>
<tr>
<td>10.0</td>
<td>1.74</td>
<td></td>
</tr>
<tr>
<td>14.1</td>
<td>1.73</td>
<td></td>
</tr>
<tr>
<td>18.7</td>
<td>1.78</td>
<td></td>
</tr>
<tr>
<td>24.8</td>
<td>1.75</td>
<td></td>
</tr>
</tbody>
</table>

change in enthalpy:

\[
\Delta H_{OW}/(\text{kJ mol}^{-1}) = 5.2
\]

(0.0 to 10.4)

enthalpy of transfer

\[
\Delta H_{oct}/(\text{kJ mol}^{-1}) = 2.5
\]

(−2.7 to 7.7)
FIGURE 5.1.1.6.4 Logarithm of $K_{OW}$ versus reciprocal temperature for 1,1-dichloroethane.
5.1.1.7 1,2-Dichloroethane

Common Name: 1,2-Dichloroethane
Synonym: ethylene chloride, ethylene dichloride, glycol dichloride, sym-dichloroethane, Dutch oil, EDC
Chemical Name: 1,2-dichloroethane
CAS Registry No: 107-06-2
Molecular Formula: C\(_2\)H\(_4\)Cl\(_2\), CH\(_2\)ClCH\(_2\)Cl
Molecular Weight: 98.959
Melting Point (°C):
\(-35.7\) (Lide 2003)
Boiling Point (°C):
85.3 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
1.2531, 1.2458 (20°C, 25°C, Dreisbach 1959; Dean 1985)
1.25209, 1.24637 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
78.0 (calculated-density, Wang et al. 1992)
93.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
35.15, 32.02 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
1.982 (calculated, Dreisbach 1959)
2.112 (quoted, Riddick et al. 1986)
Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
8690* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
8650 (shake flask-interferometer, Gross 1929)
8720, 9000 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
8696 (volumetric method, Wright & Schaffer 1932)
8490* (20°C, shake flask, measured range 0–56°C, Van Arkel & Vles 1936)
8620 (Seidell 1940)
8400 (data presented in graph, temp range 0–70°C, McGovern 1943; Horvath 1982)
8610* (shake flask-GC, temp range 0–80°C, Walraevens et al. 1974)
\log [S/(mol/L)] = 2070/(T/K) – 15.369 + 0.0247·(T/K); temp range 0–80°C (Walraevens et al. 1974)
8800 (shake flask-GC, McConnell et al. 1975)
8800 (20°C, Pearson & McConnell 1975)
8570, 8390, 10250 (3, 20, 34°C, shake flask-GC/ECD, Chiou & Freed 1977)
8450 (shake flask-GC, Chiou et al. 1979)
8630 (20°C, recommended, Sørensen & Arit 1979)
7987 (shake flask-LSC, Banerjee et al. 1980)
10600 (shake flask-titration, Coca & Diza 1980)
11000 (shake flask-titration/turbidity, Coca et al. 1980)
8000 (shake flask-LSC, Veith et al. 1980)
8608* (summary of literature data, temp range 0–80°C, Horvath 1982)
3506 (30°C, shake flask-headspace-GC, McNally & Grob 1984)
8044 (calculated-UNIFAC activity coeff., Banerjee 1985)
8100 (Dean 1985, Riddick et al. 1986)
8782, 9102, 9960 (20, 35, 50°C, infinite dilution activity coeff. γ\(^{-}\)-GC, Barr & Newsham 1987)
7200** (19.7°C, shake flask-GC/TC, measured range 0–80°C, Stephenson 1992)
8500, 9013, 9163 (20, 30, 40°C, infinite dilution activity coeff. γ\(^{-}\)-GC, Tse et al. 1992)
Henry’s Law Constant (Pa m$^3$/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

<table>
<thead>
<tr>
<th>Temperature Range</th>
<th>Equation</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>25°C</td>
<td>log (P/mmHg) = 7.18431 – 1358.5/(252.0 + t°C); temp range 6–161°C</td>
<td>Antoine eq. for liquid state, Dreisbach 1959</td>
</tr>
<tr>
<td>25°C</td>
<td>log (P/mmHg) = 14.142372 – 2896.480/(T/K) – 52.506; temp range 301.9–357.69 K</td>
<td>vapor-liquid equilibrium VLE data, Gutsche &amp; Knapp 1982</td>
</tr>
<tr>
<td>0°C – 100°C</td>
<td>log (P/mmHg) = 48.4226 – 3.1803 × 10$^2$/(T/K) – 15.37-log (T/K) + 7.2935 × 10$^{-3}$/(T/K)$^2$; temp range 237–365 K</td>
<td>vapor pressure eq., Yaws 1994</td>
</tr>
</tbody>
</table>

Henry’s Law Constant 

- 133.1 (exptl., 1/K$_{AW}$ (C$_W$/C$_A$), Hine & Mookerjee 1975)
- 92.3 (calculated-C$_W$/C$_A$, McConnell et al. 1975; Peason & McConnell 1975)
Halogenated Aliphatic Hydrocarbons

99.0, 123.9 (exptl., calculated-P/C, Dilling 1977)
111.3 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
174* (27.0°C, equilibrium cell-conc ratio-GC/FID, measured range 1.0–27.0°C, Leighton & Calo 1981)
\[ \ln (k_{HF}/\text{atm}) = 18.51 – 3482/(T/K); \text{temp range:} 1.0–23.0°C \] (equilibrium cell-conc ratio, Leighton & Calo 1981)
110 (recommended, Mackay & Shi 1981)
111.5 (gas stripping-GC, Warner et al. 1987)
143* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
\[ \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = –1.371 – 1522/(T/K) \] (EPICS measurements, Ashworth et al. 1988)
92.0 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
70.8 (computed value, Yaws et al. 1991)
101, 152, 182 (20, 30, 40°C, infinite dilution activity coeff. \( \gamma^\infty \)-GC, Tse et al. 1992)
110, 185, 319 (20, 35, 50°C, activity coeff. \( \gamma^\infty \)-differential pressure transducer, Wright et al. 1992)
122.5 \( (\gamma^\infty \text{ from gas stripping-GC, Li et al. 1993}) \)
5.30, 8.99 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
92.1 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
95.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)
185.2 (EPICS-GC, Ayuttaya et al. 2001)
102 (20°C, selected from reported experimentally determined values, Staudinger & Roberts 2001)
\[ \log K_{AW} = 4.434 – 1705/(T/K) \] (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \) at 25°C or as indicated. Additional data at other temperatures designated *
are compiled at the end of this section:

1.48 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979, 1987)
1.45 (shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)
1.58, 1.54 (calculated-octanol and water mutual solubility not considered, calculated-octanol and water mutual solubility considered, Arbuckle 1983)
1.44 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
1.48 (recommended, Sangster 1993)
1.55 (calculated-from activity coefficients, Tse & Sandler 1994)
1.51* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
1.48 (recommended, Hansch et al. 1995)
1.46* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
2.78 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.30 (bluegill sunfish, Barrows et al. 1980)
0.301 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
0.954 (microorganisms-water, calculated-\( K_{OW} \), Mabey et al. 1982; quoted, Ma et al. 1990)
0.30 (bluegill sunfish, Davies & Dobbs; quoted, Sabl 1987; Ma et al. 1990)

Sorption Partition Coefficient, log \( K_{OC} \) at 25°C or as indicated:
1.28 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.51 (soil, quoted from Chiou et al. 1979, Karickhoff 1981)
1.06, 1.19, 1.48 \( \text{estimated-} K_{OW} \) estimated-S and mp, estimated-S, Karickhoff 1981)
2.18 \( \text{estimated-} K_{OW} \), Lyman et al. 1982)
1.15 (sediment-water, calculated-\( K_{OW} \), Mabey et al. 1982)
1.09 (BUA 1987; quoted, Brüggemann et al. 1991)
Sorption Partition Coefficient, $\log K_{OM}$:

- 1.28, 1.50 (quoted, calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{\frac{1}{2}}$:

- Volatilization: estimated experimental half-life of volatilization from aqueous solution of 1 mg/L to be (28 ± 1) min when stirred at 200 rpm in water at approx. 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
- Evaporation $t_{\frac{1}{2}}$(exptl) = 28.0 min, $t_{\frac{1}{2}}$(calc) = 4.5 min, 24.5 min from water (Dilling 1977);
- Rate of evaporation $k = 2.4 \text{ g m}^{-2} \text{s}^{-1}$ (Environment Canada 1984);
- $t_{\frac{1}{2}} = 90 \text{ d}$, estimated volatilization loss from soil (Jury et al. 1990).

- Photolysis: photocatalyzed mineralization by the presence of TiO$_2$ with the rate of 1.1 ppm/min per gram of catalyst (Ollis 1985)

- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (2.2 \pm 0.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-laser magnetic resonance, Howard & Eversen 1976b; quoted, Callahan et al. 1979)
  - $k_{OH} = 0.1 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ and $t_{\frac{1}{2}} = 234 \text{ h}$ (Radding et al. 1977; quoted, Callahan et al. 1979)
  - $k_{OH} = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with residence time of 53 d, loss of 1.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
  - $k_{OH} = 1.3 \times 10^{13} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated, at 300 K (Lyman 1982)
  - $k < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k < 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radicals at 25°C (Mabey et al. 1982)
  - Photooxidation $t_{\frac{1}{2}} = 292–2917 \text{ h}$, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)
  - $k_{aq.} \leq 0.05 \text{ M}^{-1} \text{ h}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with a $t_{\frac{1}{2}} \geq 8 \text{ d}$ at pH 7 (Yao & Haag 1991).

- Hydrolysis:
  - $k = 5 \times 10^{-13} \text{ s}^{-1}$ with a max. $t_{\frac{1}{2}} = 50,000 \text{ yr}$ at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979);
  - $k = 1.80 \times 10^{-9} \text{ h}^{-1}$ for neutral process (Mabey et al. 1982; quoted, Ma et al. 1990)
  - $t_{\frac{1}{2}}$(abiotic) or $t_{\frac{1}{2}}$(dehydrohalogenation) = 50 months (Mabey et al. 1983; quoted, Olsen & Davis 1990)
  - $k$(neutral) = .63 yr$^{-1}$ with first-order $t_{\frac{1}{2}} = 1.1 \text{ yr}$ (Kollig et al. 1987; quoted, Howard et al. 1991)
  - $k = 1.1 \times 10^{-6} \text{ h}^{-1}$ at pH 7 and 25°C with calculated $t_{\frac{1}{2}} = 72 \text{ yr}$ (Jeffers et al. 1989; quoted, Ellington 1989; Brüggemann et al. 1991)
  - $t_{\frac{1}{2}} = 400 \text{ d}$ at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: relatively undegradable (Lyman et al. 1982; quoted, Brüggemann et al. 1991)

- $k < 1.4 \times 10^{-5} \text{ min}^{-1}$ disappearance rate in sediment-water sample, with $t_{\frac{1}{2}} > 35 \text{ d}$ (Jafvert & Wolfe 1987)
- $t_{\frac{1}{2}}$(aq. aerobic) = 2400–4320 h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991)
- $t_{\frac{1}{2}}$(aq. anaerobic) = 9600–17280 h (Howard et al. 1991)
- $t_{\frac{1}{2}} > 60 \text{ d}$ (Olsen & Davis 1990)
- $t_{\frac{1}{2}}$(aerobic) = 100 d, $t_{\frac{1}{2}}$(anaerobic) = 400 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).
residence time of 53 d, loss of 1.9% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981).

\[ t_{1/2} = 292–2917 \text{ h}, \] based on photooxidation half-life in air from measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);
estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: \[ t_{1/2} = 2400–4320 \text{ h}, \] based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991);
\[ t_{1/2} > 35 \text{ d} \] in sediment-water sample (Jafvert & Wolfe 1987)
\[ t_{1/2}\text{(aerobic)} = 100 \text{ d}, \] \[ t_{1/2}\text{(anaerobic)} = 400 \text{ d} \] in natural waters (Capel & Larson 1995)
measured rate constant \( k \leq 0.05 \text{ M}^{-1} \text{s}^{-1} \) for direct reaction with ozone in water at pH 2 and 21°C, with \[ t_{1/2} \geq 8 \text{ d} \] at pH 7 (Yao & Haag 1991).

Ground water: \[ t_{1/2} = 2400–8640 \text{ h}, \] based on unacclimated grab sample of aerobic soil from ground water aquifers and estimated aqueous aerobic biodegradation half-life (Wilson et al. 1983; Howard et al. 1991).

Sediment: \[ t_{1/2} > 35 \text{ d} \] in Bar-H sediment-water sample (Jafvert & Wolfe 1987)
Soil: \[ t_{1/2} = 10–50 \text{ d} \] (Ryan et al. 1988);
\[ t_{1/2} = 90 \text{ d}, \] estimated volatilization loss from soil (Jury et al. 1990);
\[ t_{1/2} = 2400–4320 \text{ h}, \] based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: \[ 1 < t_{1/2} < 2 \text{ d} \] in tissues of bluegill sunfish (Barrows et al. 1980);
\[ t_{1/2} = 10–50 \text{ d}, \] subject to plant uptake via volatilization (Ryan et al. 1988).

### TABLE 5.1.1.7.1
Reported aqueous solubilities of 1,2-dichloroethane at various temperatures

\[
\log [S/(\text{mol/L})] = -A + 2070/(T/\text{K}) + B(T/\text{K}) \tag{1}
\]
\[
S/(\text{wt%}) = 0.888 - 4.0468 \times 10^{-3} \cdot (t/\text{°C}) + 9.37388 \times 10^{-5} \cdot (t/\text{°C})^2 + 9.8465 \times 10^{-7} \cdot (t/\text{°C})^3 \tag{2}
\]
\[
S/(\text{wt%}) = 17.9147 - 0.11684 \cdot (T/\text{K}) + 2.0003 \times 10^{-4} \cdot (T/\text{K})^2 \tag{3}
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>9220</td>
<td>0</td>
<td>8370</td>
<td>10</td>
<td>8520</td>
<td>0</td>
<td>8880</td>
</tr>
<tr>
<td>10</td>
<td>8650</td>
<td>20</td>
<td>8490</td>
<td>20</td>
<td>8490</td>
<td>10</td>
<td>8579</td>
</tr>
<tr>
<td>20</td>
<td>8690</td>
<td>36</td>
<td>8950</td>
<td>25</td>
<td>8610</td>
<td>20</td>
<td>8524</td>
</tr>
<tr>
<td>30</td>
<td>8904</td>
<td>56</td>
<td>10300</td>
<td>30</td>
<td>8800</td>
<td>25</td>
<td>8608</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>40</td>
<td>9440</td>
<td>30</td>
<td>8775</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>10460</td>
<td>40</td>
<td>9391</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
<td>11920</td>
<td>50</td>
<td>10430</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>70</td>
<td>13950</td>
<td>60</td>
<td>11951</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>80</td>
<td>16720</td>
<td>70</td>
<td>14014</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>80</td>
<td>16678</td>
<td>80</td>
<td>16678</td>
</tr>
</tbody>
</table>

Gross & Saylor 1931

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>8720</td>
<td>eq. 1</td>
<td>S/(mol/L)</td>
<td>A 15.369</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>9000</td>
<td>eq. 1</td>
<td>S/wt%</td>
<td>B 0.0247</td>
<td></td>
</tr>
</tbody>
</table>

*Data calculated by Horvath 1982

(Continued)
### TABLE 5.1.1.7.1 (Continued)

2. 

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8782</td>
<td>0</td>
<td>8200</td>
<td>20</td>
<td>8500</td>
<td>20</td>
<td>9400</td>
</tr>
<tr>
<td>35</td>
<td>9102</td>
<td>9.3</td>
<td>7700</td>
<td>35</td>
<td>9013</td>
<td>35</td>
<td>9209</td>
</tr>
<tr>
<td>50</td>
<td>9960</td>
<td>19.7</td>
<td>7200</td>
<td>50</td>
<td>9835</td>
<td>50</td>
<td>9835</td>
</tr>
</tbody>
</table>

3. 

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>eq. 2</th>
<th>S/wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>9240</td>
<td>40</td>
<td>9410</td>
<td>80</td>
<td>15990</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>8910</td>
<td>45</td>
<td>9890</td>
<td>85</td>
<td>17270</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>8680</td>
<td>50</td>
<td>10460</td>
<td>90</td>
<td>18640</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>8550</td>
<td>55</td>
<td>11130</td>
<td>95</td>
<td>20110</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>8520</td>
<td>60</td>
<td>11900</td>
<td>100</td>
<td>21680</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>8600</td>
<td>65</td>
<td>12780</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>8770</td>
<td>70</td>
<td>13750</td>
<td>eq. 2</td>
<td>S/wt%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>9040</td>
<td>75</td>
<td>14820</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.7.1** Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for 1,2-dichloroethane.
### TABLE 5.1.1.7.2

Reported vapor pressures of 1,2-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{(C + t/°C)} \quad (2) \\
\log P = A - \frac{B}{(C + T/K)} \quad (3) \\
\log P = A - \frac{B}{(T/K)} - C\log (T/K) \quad (4)
\]

**Pearce & Peters 1929**  
**Stull 1947**  
**Gutsche & Knapp 1982**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–30.82</td>
<td>427</td>
<td>–44.5</td>
<td>133.3</td>
<td>28.75</td>
<td>12530</td>
</tr>
<tr>
<td>–24.92</td>
<td>613</td>
<td>–24.0</td>
<td>666.6</td>
<td>38.65</td>
<td>19521</td>
</tr>
<tr>
<td>–19.32</td>
<td>860</td>
<td>–13.6</td>
<td>1333</td>
<td>46.39</td>
<td>27004</td>
</tr>
<tr>
<td>–15.02</td>
<td>1093</td>
<td>–2.40</td>
<td>2666</td>
<td>51.72</td>
<td>33373</td>
</tr>
<tr>
<td>–10.42</td>
<td>1547</td>
<td>10.0</td>
<td>5333</td>
<td>56.63</td>
<td>40285</td>
</tr>
<tr>
<td>–5.12</td>
<td>2120</td>
<td>18.1</td>
<td>7999</td>
<td>60.79</td>
<td>47009</td>
</tr>
<tr>
<td>0.070</td>
<td>2800</td>
<td>29.4</td>
<td>13332</td>
<td>64.19</td>
<td>53158</td>
</tr>
<tr>
<td>5.09</td>
<td>3760</td>
<td>45.7</td>
<td>26664</td>
<td>67.62</td>
<td>60006</td>
</tr>
<tr>
<td>10.07</td>
<td>4893</td>
<td>64.0</td>
<td>53329</td>
<td>70.24</td>
<td>65669</td>
</tr>
<tr>
<td>15.52</td>
<td>6546</td>
<td>82.4</td>
<td>101325</td>
<td>73.85</td>
<td>74207</td>
</tr>
<tr>
<td>20.21</td>
<td>8279</td>
<td></td>
<td></td>
<td>76.36</td>
<td>80633</td>
</tr>
<tr>
<td>25.25</td>
<td>10639</td>
<td></td>
<td>–35.3</td>
<td>78.67</td>
<td>86926</td>
</tr>
<tr>
<td>30.23</td>
<td>13452</td>
<td></td>
<td></td>
<td>80.80</td>
<td>93115</td>
</tr>
<tr>
<td>35.24</td>
<td>16839</td>
<td></td>
<td></td>
<td>82.74</td>
<td>98997</td>
</tr>
<tr>
<td>39.79</td>
<td>20425</td>
<td></td>
<td></td>
<td>84.54</td>
<td>104743</td>
</tr>
<tr>
<td>45.13</td>
<td>25544</td>
<td></td>
<td></td>
<td>eq. 3</td>
<td>P/kPa</td>
</tr>
<tr>
<td>51.12</td>
<td>31304</td>
<td></td>
<td></td>
<td>A</td>
<td>14.142372</td>
</tr>
<tr>
<td>55.22</td>
<td>37997</td>
<td></td>
<td></td>
<td>B</td>
<td>2896.480</td>
</tr>
<tr>
<td>60.28</td>
<td>45969</td>
<td></td>
<td></td>
<td>C</td>
<td>52.506</td>
</tr>
<tr>
<td>65.27</td>
<td>55035</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>70.27</td>
<td>65448</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>75.36</td>
<td>77220</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.43</td>
<td>91046</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>85.45</td>
<td>105938</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>91.03</td>
<td>124603</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>bp/°C</td>
<td>84.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \Delta H_v/(kJ mol^{-1}) = 32.41 \text{ at bp} \]

vapor pressure eq. see ref.
**TABLE 5.1.1.7.3**
Reported Henry's law constants of 1,2-dichloroethane at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \quad (1) \\
\ln \left(1/K_{AW}\right) &= A - B/(T/K) \quad (2) \\
\ln H &= A - B/(T/K) \quad (3) \\
K_{AW} &= A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)
\end{align*}
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>55.85</td>
<td>10</td>
<td>118.6</td>
<td>2.0</td>
<td>32.03</td>
</tr>
<tr>
<td>1.3</td>
<td>56.34</td>
<td>15</td>
<td>131.7</td>
<td>6.0</td>
<td>42.47</td>
</tr>
<tr>
<td>11.0</td>
<td>84.92</td>
<td>20</td>
<td>148.95</td>
<td>10.0</td>
<td>39.55</td>
</tr>
<tr>
<td>21.0</td>
<td>125.6</td>
<td>25</td>
<td>142.87</td>
<td>18.2</td>
<td>75.4</td>
</tr>
<tr>
<td>22.0</td>
<td>139.7</td>
<td>30</td>
<td>176.3</td>
<td>25.0</td>
<td>102.1</td>
</tr>
<tr>
<td>27.2</td>
<td>174.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>119.3</td>
<td>eq. 4 H/(atm m³/mol)</td>
<td>eq. 1 K_{AW}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 3 H/atm</td>
<td>A = -1.371</td>
<td>A = 11.377</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>16.05</td>
<td>B</td>
<td>1522</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3539</td>
<td>B</td>
<td>4329</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Leighton & Calo 1981
Ashworth et al. 1988
Dewulf et al. 1995

**FIGURE 5.1.1.7.2** Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloroethane.
FIGURE 5.1.1.7.3 Logarithm of Henry’s law constant versus reciprocal temperature for 1,2-dichloroethane.

### TABLE 5.1.1.7.4
Reported octanol-water partition coefficients of 1,2-dichloroethane at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
<th>t/°C</th>
<th>log K_{OW}</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.51</td>
<td>2.2</td>
<td>1.43</td>
</tr>
<tr>
<td>35</td>
<td>1.51</td>
<td>4.0</td>
<td>1.46</td>
</tr>
<tr>
<td>50</td>
<td>1.53</td>
<td>10.0</td>
<td>1.47</td>
</tr>
<tr>
<td></td>
<td></td>
<td>14.1</td>
<td>1.44</td>
</tr>
<tr>
<td></td>
<td></td>
<td>18.7</td>
<td>1.50</td>
</tr>
<tr>
<td></td>
<td></td>
<td>24.8</td>
<td>1.46</td>
</tr>
</tbody>
</table>

change in enthalpy:  
ΔH_{ow}/kJ mol⁻¹ = 3.3  
(−2.1 to 8.6)

enthalpy of transfer  
ΔH_{oct}/kJ mol⁻¹ = 0.2  
(−5.2 to 5.5)
**FIGURE 5.1.1.7.4** Logarithm of $K_{OW}$ versus reciprocal temperature for 1,2-dichloroethane.
5.1.1.8 1,1,1-Trichloroethane

Common Name: 1,1,1-Trichloroethane
Synonym: methyl chloroform, chlorotene, Genklene, Baltana
Chemical Name: 1,1,1-trichloroethane
CAS Registry No: 71-55-6
Molecular Formula: \( \text{CH}_3\text{CCl}_3 \)
Molecular Weight: 133.404
Melting Point (°C):
-30.01  (Lide 2003)
Boiling Point (°C):
74.09   (Lide 2003)
Density (g/cm\(^3\)) at 20°C:
1.3390  (Dreisbach 1961; Horvath 1982; Weast 1982–83; McNally & Grob 1984)
1.3381, 1.3299  (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
99.0, 52.0  (calculated-density, intrinsic volume-van der Waals method, Abernethy et al. 1988)
100.0  (calculated-density, Wang et al. 1992)
114.5  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
32.74, 29.74  (25°C, bp, Dreisbach 1961)
32.39, 29.708  (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{ fus } \) (kJ/mol):
2.35  (Riddick et al. 1986)
Entropy of Fusion, \( \Delta S_{ fus } \) (J/mol K):

Fugacity Ratio at 25°C, \( F \): 1.0  (Suntio et al. 1988)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1320*  (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
1304  (Seidell 1940)
1490*  (shake flask-GC, measured range 10–80°C, Walraevens et al. 1974)
\[ \log \left[ \frac{S}{(\text{mol/L})} \right] = \frac{2070}{(T/K)} - 14.860 + 0.020 \cdot (T/K) \] temp range 2630353 K (shake flask, Walraevens et al. 1974)
480  (20°C, shake flask-GC, Pearson & McConnell 1975; McConnell et al. 1975)
880, 720  (1.5, 25°C, average literature values, Dilling 1977)
1360  (shake flask, Chiou et al. 1979)
1320  (20°C, recommended, Sørensen & Arit 1979)
100  (shake flask-titration, Coca & Diaz 1980)
1334  (shake flask-LSC, Banerjee et al. 1980)
1150, 1200  (23.5°C, elution chromatography, Schwarz 1980)
1850*  (20°C, elution chromatography, measured range 10–30°C, Schwarz & Miller 1980)
1334; 278.7  (shake flask-LSC; calculated-f const., Veith et al. 1980)
1260  (calculated-group contribution as per Irann 1965, Horvath 1982)
1485*  (summary of literature data, temp range 0–80°C, Horvath 1982)
3200  (calculated-UNIFAC activity coeff., Arbuckle 1983)
479.8  (30°C, headspace-GC, McNally & Grob 1984)
1334  (calculated-UNIFAC activity coeff., Banerjee 1985)
1320  (20°C, selected, Riddick et al. 1986)
1310, 1194, 1267 (20, 35, 50°C, infinite dilution activity coeff. \( \gamma \)-GC, Barr & Newsham 1987)
1252  (23–24°C, shake flask-GC, Broholm et al. 1992)
700*  (20.2°C, shake flask-GC/TC, measured range 0–71.5°C, Stephenson 1992)
1260, 1353, 1370 (20, 30, 40°C, activity coeff. γ - differential pressure transducer, Wright et al. 1992)
1413, 1353, 1370 (20, 30, 35, 40°C, infinite dilution activity coeff. γ – GC, Tse et al. 1992)
2935, 3228, 3536, 3749 (20, 30, 35, 40°C, infinite dilution activity coeff. γ – UNIFAC, Tse et al. 1992)
1758 (γ∞ from gas stripping-GC, Li et al. 1993)
1250 (shake flsk-GC, Broholm & Feenstra 1995)
1380 (20°C, activity coeff. γ∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
1290* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 1.09092 – 6.52776 × 10–3·(T/K) + 1.10747 × 10–5·(T/K)2, temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
12159* (17.68°C, static method-Hg manometer, measured range 268–290 K, Rubin et al. 1944)
log (P/cmHg) = 6.92013 – 1729/(T/K); temp range 268–290 K (Hg manometer, Rubin et al. 1944)
16190* (interpolated from Antoine eq. regression, temp range –52 to 74.1°C, Stull 1947)
16100 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.94983 – 1217.0/(225.0 + t°C); temp range –3 to 111°C (Antoine eq. for liquid state, Dreisbach 1961)
16170 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 8012.7/(T/K)] + 7.955902; temp range –52 to 74.1°C (Antoine eq., Weast 1972–73)
16490* (ebulliometry, measured range –77.15 to 25°C, Ambrose et al. 1975)
16490 (ebulliometry, measured –77.15 to 25°C, Boublik et al. 1984)
17800 (calculated-Antoine eq., Boublik et al. 1973, 1984)
log (P/mmHg) = 8.64344 – 2136.621/(302.769 + t°C); temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
12800 (20°C, Pearson & McConnell 1975; McConnell et al. 1975)
17800, 16490 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.78612 – 2147.034/(303.568 + t°C); temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.13297 – 1260.034/(231.327 + t/°C); temp range –77.2 to 25°C (Antoine eq. from reported exptl. data of Ambrose et al. 1973, Boublik et al. 1984)
log (P/mmHg) = 8.6434 – 2136.6/(302.8 + t°C); temp range –6 to 17°C (Antoine eq., Dean 1985, 1992)
16490 (selected, Riddick et al. 1986)
log (P/kPa) = 5.98755 – 1182.527(222.594 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
16490 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.98755 – 1182.527/(–50.256 + T/K); temp range; 295–372 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.00452 – 1193.604/(–48.734 + T/K); temp range 349–408 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.36873 – 1474.394/(–8.08 + T/K); temp range 399–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)
16530, 960 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
13150, 20520, 25300, 30940 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 36.5468 – 2.821 × 103/(T/K) – 10.205·log (T/K) – 2.6369 × 10 –9·(T/K) + 3.7075 × 10–6·(T/K)2; temp range 243–545 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1638 (calculated as 1/Kaw, CA/W, reported as exptl., Hine & Mookerjee 1975)
3433 (20°C, McConnell et al. 1975)
2800, 2875 (exptl., calculated-P/C, Dilling 1977)
2025 (20°C, batch stripping-GC, Mackay et al. 1979)
730 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
log (kH/atm) = 9.39 – 1992.95/(T/K), (least-square regression of data from lit., Kavanaugh & Trussell 1980)
ln (k_H/atm) = 21.68 – 4375/(T/K); temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1520  (20°C, batch air stripping, Munz & Roberts 1982)

1319* (multiple equilibrium technique-GC, temp range 5–33°C, Hunter-Smith et al. 1983)

ln K_{AW} = 9.15 – 2915/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

ln K_{AW} = 13.04 – 3905/(T/K); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)

ln \[H/(atm m^3/mol)\] = 10.21 – 4262/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)

498.5 (adsorption isotherm, Urano & Murata 1985)

498.5 (gas stripping-GC, Warner et al. 1987)

1345, 1413* (20, 25°C, EPICS-GC/FID, measured range 9.6–24.6°C, Gossett 1987)


K_{AW} = 0.204 + 0.0182·(T/K) + 0.000173·(T/K)^2; temp range 0–35°C (vapor-liquid equilibrium-GC with additional lit. data, Turner et al. 1996)

1280 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)

1614, 1750, 1415; 1380 (direct calculated method, gas-phase EPICS method, liquid-phase EPICS method; quoted lit. Chiang et al. 1998)

2.17 (Tute 1971)

2.49 (shake flask, Hansch & Leo 1979; Hansch & Leo 1985)

2.47 (shake flask-LSC, Banerjee et al. 1980)

2.47 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)

2.35, 2.29 (calculated-UNIFAC with octanol and water mutual solubility not considered, calculated-UNIFAC with octanol and water mutual solubility considered, Arbuckle 1983)

1.96 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)

2.49 (recommended, Sangster 1993)

2.60 (calculated-activity coefficients, Tse & Sandler 1994)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.47* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
2.20* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log $K_{OA}$:
2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.40 (calculated-$K_{OW}$, Veith et al. 1979; Veith et al. 1980)
0.954 (bluegill sunfish, Veith et al. 1980)
0.954 (bluegill sunfish, Barrows et al. 1980)
1.908 (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)
0.950 (bluegill sunfish, Veith & Kosian 1982)
1.70 (calculated-MCI $\chi$, Koch 1983)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
2.02 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
2.25 (quoted from Chiou et al. 1979, Karickhoff 1981, 1985)
2.08, 2.04, 2.02 (estimated-$K_{OW}$, estimated-S and mp, estimated-S, Karickhoff 1981)
2.182 (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
2.20 (soil, best estimate, Karickhoff 1985)
1.70 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
2.26 (20°C, soil, Chiou et al. 1988)
1.65 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
2.22 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
3.02 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
2.053 (soil, selected, Jury et al. 1990)
1.95, 1.98, 1.99, 2.01, 1.98, 2.03 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
3.20 (soil, calculated-universal solvation model, Winget et al. 2000)
2.16 (soil: organic carbon $OC \geq 0.1\%$, average, Delle Site 2001)

Sorption Partition Coefficient, log $K_{OM}$:
2.02, 1.55 (quoted, calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
Volatilization: evaporation $t_\frac{1}{2}$ (exptl) = 21 min, $t_\frac{1}{2}$ (calc) = 0.34 min from water (Dilling et al. 1975)
$\text{t}_\frac{1}{2}$ (exptl) = (20 ± 3) min at 25°C for an aqueous solution of 1 mg L$^{-1}$ when stirred at 200 rpm in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
Evaporation $t_\frac{1}{2}$ (exptl) = (17.3–24.9) min, $t_\frac{1}{2}$ (calc) = 0.19 min, 23.7 min at 20–25°C, and $t_\frac{1}{2}$ = 30.2 min at 15°C from water (Dilling 1977);
estimated $t_\frac{1}{2}$ = (3.7 h) from water (Thomas 1982);
$k = 0.029 d^{-1}$, $t_\frac{1}{2}$ = 24 d in spring at 8–16°C, $k = 0.058 d^{-1}$, $t_\frac{1}{2}$ = 12 d in summer at 20–22°C, $k = 0.063 d^{-1}$, $t_\frac{1}{2}$ = 11 d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.60 d^{-1}$, $t_\frac{1}{2}$ = 11.5 d with HgCl$_2$, and $k = 0.072 d^{-1}$, $t_\frac{1}{2}$ = 9.6 d without HgCl$_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);
estimated $t_\frac{1}{2}$ = 365 d for volatilization loss from soil to be 365 d (Jury et al. 1990).
Photolysis: not expected to be important (Howard et al. 1991).
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3^-$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$k_{OH} = 3.36 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a troposphere life time of 1.1 yr at 298 K (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)
$k_{OH} = (1.5 \pm 0.3) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (discharge flow-resonance fluorescence, Howard & Evenson 1976b)
**Halogenated Aliphatic Hydrocarbons**

\[ k_{OH}^* = (2.19 \pm 0.26) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, measured range 275–405 K, with calculated lifetime of 3.8–6.0 yr in troposphere (discharge flow system-resonance fluorescence, Chang & Kaufman 1977)

\[ k_{OH} = (1.59 \pm 0.16) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K with lifetime of 13 yr (flash photolysis-resonance fluorescence, Watson et al. 1977; quoted, Callahan et al. 1979; Altshuller 1980)

\[ k_{OH}^* = (1.06 \pm 0.09) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 293 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

\[ k_{OH} = (1.08 \pm 0.20) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 296 K, measured range 222–363 K (flash photolysis-resonance fluorescence, Kurylo et al. 1979)

\[ k_{OH} = 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \], with an estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

\[ k = 9.0 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \], estimated at 300 K (Lyman 1982)

\[ k << 360 \text{ M}^{-1} \text{ hr}^{-1} \] for singlet oxygen and 1.0 M\(^{-1}\) hr\(^{-1}\) for peroxy radical at 25°C (Mabey et al. 1982)

Photooxidation \( t_{1/2} \) = 5393–53929 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

\[ k_{OH}^{(calc)} = 1.3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \], \( k_{OH}^{(obs.)} = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (SAR [structure-activity relationship], Atkinson 1987)

\[ k_{OH}^* = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (recommended, Atkinson 1989)

\[ k_{OH} = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Prinn et al. 1987; quoted, Bunce et al. 1991)

\[ k_{OH}^{(aq.)} \leq 0.012 \text{ M}^{-1} \text{ s}^{-1} \] for direct reaction with ozone in water at pH 2 and 22°C, with \( t_{1/2} \geq 32 \text{ d} \) at pH 7 (Yao & Haag 1991).

**Hydrolysis:**

\[ k = 0.12 \text{ month}^{-1} \] with \( t_{1/2}^{(exptl.)} = 6 \text{ months} \) at pH 7 and 25°C (Dilling et al. 1975; quoted, Callahan et al. 1979; Mabey et al. 1979; Neely 1985)

\[ k = 0.96 \text{ yr}^{-1} \] at pH 7 and 25°C with a first-order hydrolysis \( t_{1/2} = 0.73 \text{ yr} \) (Kollig et al. 1987)

\[ k = (1.93 \pm 0.40) \times 10^{-8} \text{ s}^{-1} \] in distilled water contained 0.1% w/w CH\(_2\)O as sterilant with 39% conversion,

\[ k = (2.04 \pm 0.47) \times 10^{-8} \text{ s}^{-1} \] in autoclaved distilled water with 40% conversion and

\[ k = (1.80 \pm 0.90) \times 10^{-8} \text{ s}^{-1} \] in sediment contained 0.1% w/w CH\(_2\)O as sterilant with 25% conversion at 25°C, calculated \( t_{1/2} = 350 \text{ d} \) at 25°C (Haag & Mill 1988)

\( t_{1/2} = 6 \text{ months} \), abiotic hydrolysis or dehydrohalogenation half-life (Olsen & Davis 1990)

\( t_{1/2} = 0.73 \text{ yr} \), based on reported rate constant at pH 7 at 25°C (Howard et al. 1991)

**Biodegradation:**

\[ k = 0.043 \text{ d}^{-1} \] in fresh water plus sediment incubated under anaerobic conditions (Wood et al. 1981; quoted, Klecka 1985)

\( t_{1/2}^{(aq. \text{, aerobic})} = 3360–6852 \text{ h} \), based on unacclimated aerobic seawater grab sample data and sub-soil sample data from a ground water aquifer (Pearson & McConnell 1975; Wilson et al. 1983; quoted, Howard et al. 1991)

\( t_{1/2}^{(aq. \text{, anaerobic})} = 13440–26208 \text{ h} \), based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991)

**Biotransformation:**

**Bioconcentration, Uptake (k\(_1\)) and Elimination (k\(_2\)) Rate Constants or Half-Lives:**

**Half-Lives in the Environment:**

Air: tropospheric \( t_{1/2} = 26 \text{ wk} \), when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

Disappearance \( t_{1/2} = 2.4–24 \text{ h} \) from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

Estimated troposphere residence time of 1.1 yr for reaction with OH radical (CEQ 1975)

Estimated N. troposphere residence time of 7.2 yr by one compartment non-steady state model (Singh et al. 1978)

Estimated troposphere residence time of 8–10 yr by two compartment non-steady state model (Singh 1977; Singh et al. 1979)

Estimated lifetime of 8 yr in troposphere (Altshuller 1980)

Estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

Atmospheric lifetime \( \tau = 6.3 \text{ yr} \) (Prinn et al. 1987)
troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Bunce et al. 1991; estimated tropospheric lifetime of 7.8 yr and 6.1 yr by rigorous calculations (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 24$ d in the spring at 8–16°C, $t_{1/2} = 12$ d in the summer at 20–22°C, $t_{1/2} = 11$ d in the winter at 3–7°C when volatilization dominates, and $t_{1/2} = 11.5$ d and 9.6 d for experiments with and without HgCl$_2$ as poison, respectively, in September 9–15 in marine mesocosm experiment (Wakeham et al. 1983); calculated hydrolysis $t_{1/2} = 350$ d at 25°C (Haag & Mill 1988); $t_{1/2} = 3360$–6552 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) \leq 0.012$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 32$ d at pH 7 (Yao & Haag 1991).

Ground water: estimated $t_{1/2} \sim 1.0$ yr in the groundwater of the Netherlands (Zoeteman et al. 1981); $t_{1/2} = 3360$–13104 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a ground water aquifer (Howard et al. 1991; Wilson et al. 1983).

Sediment: measured $t_{1/2} = 450$ d at 25°C, based on neutral and base-catalyzed hydrolysis rates studied in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: $t_{1/2} = 365$ d, estimated volatilization loss (Jury et al. 1990); $t_{1/2} = 3360$–6552 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980).

### TABLE 5.1.1.8.1

Reported aqueous solubilities of 1,1,1-trichloroethane at various temperatures

1. **Van Arkel & Vles 1936**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1590</td>
</tr>
<tr>
<td>20</td>
<td>1320</td>
</tr>
<tr>
<td>35</td>
<td>1260</td>
</tr>
<tr>
<td>50</td>
<td>1280</td>
</tr>
</tbody>
</table>

2. **Walraevens et al. 1974**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1730</td>
</tr>
<tr>
<td>20</td>
<td>1550</td>
</tr>
<tr>
<td>30</td>
<td>1440</td>
</tr>
<tr>
<td>40</td>
<td>1390</td>
</tr>
</tbody>
</table>

3. **Schwarz & Miller 1980**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1800</td>
</tr>
<tr>
<td>20</td>
<td>1850</td>
</tr>
<tr>
<td>30</td>
<td>1590</td>
</tr>
</tbody>
</table>

4. **Horvath 1982**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1910</td>
</tr>
<tr>
<td>10</td>
<td>1707</td>
</tr>
<tr>
<td>20</td>
<td>1554</td>
</tr>
<tr>
<td>25</td>
<td>1495</td>
</tr>
<tr>
<td>30</td>
<td>1449</td>
</tr>
<tr>
<td>40</td>
<td>1390</td>
</tr>
<tr>
<td>50</td>
<td>1377</td>
</tr>
<tr>
<td>60</td>
<td>1407</td>
</tr>
<tr>
<td>70</td>
<td>1479</td>
</tr>
<tr>
<td>80</td>
<td>1592</td>
</tr>
</tbody>
</table>

**eq. 1 S/wt%**
### TABLE 5.1.1.8.1 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>activity coefficient</td>
<td>shake flask-GC</td>
<td>activity coefficient</td>
<td>recommended, IUPAC-NIST</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td></td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>20</td>
<td>1310</td>
<td>0</td>
<td>20</td>
<td>1413</td>
</tr>
<tr>
<td>35</td>
<td>1194</td>
<td>20.2</td>
<td>30</td>
<td>1392</td>
</tr>
<tr>
<td>50</td>
<td>1267</td>
<td>31.6</td>
<td>35</td>
<td>1454</td>
</tr>
<tr>
<td></td>
<td></td>
<td>41.1</td>
<td>40</td>
<td>1489</td>
</tr>
<tr>
<td></td>
<td></td>
<td>51.3</td>
<td>1060</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td></td>
<td>61.5</td>
<td>1030</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>71.5</td>
<td>1140</td>
<td>25</td>
</tr>
</tbody>
</table>

#### Wright et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1260</td>
</tr>
<tr>
<td>30</td>
<td>1353</td>
</tr>
<tr>
<td>40</td>
<td>1370</td>
</tr>
</tbody>
</table>

**temp range 273–323 K**

#### FIGURE 5.1.1.8.1

Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,1-trichloroethane.

© 2006 by Taylor & Francis Group, LLC
<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–5.534</td>
<td>3840</td>
<td>–52.0</td>
<td>1333</td>
<td>–77.15</td>
<td>20</td>
</tr>
<tr>
<td>–0.207</td>
<td>5160</td>
<td>–32.0</td>
<td>666.6</td>
<td>–55.15</td>
<td>100</td>
</tr>
<tr>
<td>5.12</td>
<td>6733</td>
<td>–21.9</td>
<td>1333</td>
<td>–25.85</td>
<td>1000</td>
</tr>
<tr>
<td>11.33</td>
<td>9239</td>
<td>–10.8</td>
<td>2666</td>
<td>14.15</td>
<td>10000</td>
</tr>
<tr>
<td>16.93</td>
<td>12159</td>
<td>1.6</td>
<td>5333</td>
<td>25.0</td>
<td>16490</td>
</tr>
<tr>
<td>mp/K</td>
<td>240.2</td>
<td>20.0</td>
<td>13332</td>
<td>36.2</td>
<td>53329</td>
</tr>
<tr>
<td>eq. 1</td>
<td>P/cmHg</td>
<td>54.6</td>
<td>101325</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>6.92013</td>
<td>74.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1729</td>
<td>mp°C</td>
<td>–30.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\Delta H_v/(kJ \ mol^{-1}) = 33.42$

at 286.53 K

**FIGURE 5.1.1.8.2** Logarithm of vapor pressure versus reciprocal temperature for 1,1,1-trichloroethane.
### TABLE 5.1.1.8.3
Reported Henry's law constants of 1,1,1-trichloroethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \\
\log K_{AW} = A - B/(T/K) \quad (1a) \\
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \\
\log (1/K_{AW}) = A - B/(T/K) \quad (2a) \\
\ln H = A - B/(T/K) \quad (3) \\
\log H = A - B/(T/K) \quad (4) \\
\ln (kH/\text{atm}) = A - B/(T/K) \quad (4) \\
\ln H = A - B/(T/K) + C(T/K)^2 \quad (5)
\]

1. Leighton & Calo 1981

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>541.7</td>
</tr>
<tr>
<td>1.0</td>
<td>543.3</td>
</tr>
<tr>
<td>1.2</td>
<td>555.9</td>
</tr>
<tr>
<td>2.5</td>
<td>597.9</td>
</tr>
<tr>
<td>7.0</td>
<td>763.3</td>
</tr>
<tr>
<td>10.0</td>
<td>919.2</td>
</tr>
<tr>
<td>12.0</td>
<td>1016</td>
</tr>
<tr>
<td>12.0</td>
<td>1039</td>
</tr>
<tr>
<td>12.9</td>
<td>1069</td>
</tr>
<tr>
<td>14.0</td>
<td>1190</td>
</tr>
<tr>
<td>18.0</td>
<td>1398</td>
</tr>
<tr>
<td>18.0</td>
<td>1447</td>
</tr>
<tr>
<td>18.0</td>
<td>1464</td>
</tr>
<tr>
<td>19.0</td>
<td>1511</td>
</tr>
<tr>
<td>19.2</td>
<td>1526</td>
</tr>
<tr>
<td>19.5</td>
<td>1437</td>
</tr>
<tr>
<td>24.3</td>
<td>1874</td>
</tr>
<tr>
<td>25.2</td>
<td>1995</td>
</tr>
<tr>
<td>25.3</td>
<td>2026</td>
</tr>
<tr>
<td>26.0</td>
<td>1988</td>
</tr>
<tr>
<td>26.0</td>
<td>2064</td>
</tr>
<tr>
<td>26.1</td>
<td>1958</td>
</tr>
</tbody>
</table>

\[
\ln (kH/\text{atm}) = A - B/(T/K) \\
A \quad 21.68 \\
B \quad 4375
\]

2. Kolb et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>1578</td>
</tr>
<tr>
<td>60</td>
<td>1884</td>
</tr>
<tr>
<td>70</td>
<td>2264</td>
</tr>
<tr>
<td>80</td>
<td>2488</td>
</tr>
</tbody>
</table>

\[
eq 2 \quad 1/K_{AW} \\
A \quad -2.52 \\
B \quad -950
\]

(Continued)
TABLE 5.1.1.8.3 (Continued)
3.

<table>
<thead>
<tr>
<th>Robbins et al. 1993</th>
<th>Dewulf et al. 1995</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>static headspace-GC</strong></td>
<td><strong>EPICS-GC</strong></td>
</tr>
<tr>
<td>$t/^{\circ}C$</td>
<td>$H/(Pa \ m^3/mol)$</td>
</tr>
<tr>
<td>25</td>
<td>1783</td>
</tr>
<tr>
<td>30</td>
<td>2209</td>
</tr>
<tr>
<td>40</td>
<td>2675</td>
</tr>
<tr>
<td>45</td>
<td>3597</td>
</tr>
<tr>
<td>50</td>
<td>4164</td>
</tr>
</tbody>
</table>

\[ eq. 1 \quad K_{AW} = A - \frac{\Delta H}{2.303RT} \]

A \quad 12.351
B \quad 3834

FIGURE 5.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.4
Reported octanol-water partition coefficients of 1,1,1-trichloroethane at various temperatures

<table>
<thead>
<tr>
<th>Bhatia &amp; Sandler 1995</th>
<th>Dewulf et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>relative GC-RT technique</strong></td>
<td><strong>shake flask-GC</strong></td>
</tr>
<tr>
<td>$t/^{\circ}C$</td>
<td>$\log K_{OW}$</td>
</tr>
<tr>
<td>25</td>
<td>2.47</td>
</tr>
<tr>
<td>35</td>
<td>2.50</td>
</tr>
<tr>
<td>50</td>
<td>2.52</td>
</tr>
</tbody>
</table>

enthalpy of transfer
\[ \Delta H/(kJ \ mol^{-1}) = -20.2 \]

\[ \log K_{OW} = A - \Delta H/2.303RT \]

A \quad 1.0195
\Delta H \quad -20.2
FIGURE 5.1.18.4 Logarithm of $K_{OW}$ versus reciprocal temperature for 1,1,1-trichloroethane.
5.1.1.9 1,1,2-Trichloroethane

Common Name: 1,1,2-Trichloroethane
Synonym: vinyl trichloride
Chemical Name: 1,1,2-trichloroethane
CAS Registry No: 79-00-5
Molecular Formula: CH₂ClCHCl₂
Molecular Weight: 133.404
Melting Point (°C):
  –36.3 (Lide 2003)
Boiling Point (°C):
  113.8 (Lide 2003)
Density (g/cm³ at 20°C):
  1.440 (Dreisbach 1959; Weast 1982–83; Verschueren 1983;)
  1.43931, 1.43213(20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  93.0 (calculated-density, Wang et al. 1992)
  114.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  46.77, 37.07 (25°C, bp, Dreisbach 1961)
  40.28, 34.23 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  11.543 (Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are complied at the end of this section):

3704 (volumetric method, Wright & Schaffer 1932)
4580* (shake flask, measured range 0–55°C, Van Arkel & Vles 1936)
4418 (Seidell 1940)
4400 (data presented in graph, temp range 0–70°C, McGovern 1943)
4400 (shake flask-refractive index and density, Treybal et al. 1946)
4380* (shake flask-GC, measured range 0–80°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 15.285 + 0.0230·(T/K); temp range 0–80°C (Walraevens et al. 1974)
4420 (literature average, Dilling 1977)
4500 (20°C, Verschueren 1977, 1983)
4370 (20°C, recommended, Sørensen & Arit 1979)
5100 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)
1490 (shake flask-LSC, Veith et al. 1980)
4394* (summary of literature data, temp range 0–80°C, Horvath 1982)
4365 (30°C, headspace-GC, McNally & Grob 1984)
4800 (Dean 1985)
4941, 4876, 5183 (20, 35, 50°C, infinite dilution activity coeff. γ∞-GC, Barr & Newsham 1987)
2858, 1469 (predicted-MCI γ and polarizability, Nirmalakhandan & Speece 1988)
4580* (31.3°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson 1992)
4813, 5035, 5205 (20, 30, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)
2574, 2960, 3378 (20, 30, 40°C, infinite dilution activity coeff. γ∞-UNIFAC, Tse et al. 1992)
4877, 5257, 6075 (20, 35, 50°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
4460 (20°C, activity coeff. γ∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
4590* (tentative values, temp range 0–55°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

\[ S/(\text{wt}%) = 2.89796 \times 10^{-2} - 3.48961 \times 10^{-5} \cdot (T/K), \text{ temp range 273–328 K} \] (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):

26664* (73.5°C, ebulliometry, measured range 73.5–113.5°C, Treybal et al. 1946)

3090* (Antoine eq. regression, temp range –24 to 113.9°C, Stull 1947)

19114* (49.97°C, ebulliometry, measured range 49.97–113.67°C, Dreisbach & Shrader 1949)

2998 (calculated-Antoine eq., Dreisbach 1959)

\[ \log (P/\text{mmHg}) = 6.84165 - 1262.6/(205.0 + t/°C); \text{ temp range 30–186°C} \] (Antoine eq. for liquid state, Dreisbach 1959)

3218 (calculated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P/\text{mmHg}) = [-0.2185 \times 9163.2/(T/K)] + 8.079996; \text{ temp range –24 to 113.9°C} \] (Antoine eq., Weast 1972–73)

2910 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

3066 (literature average, Dilling 1977)

2533, 4266 (20, 30°C, Verschueren 1983)

\[ \log (P/\text{mmHg}) = 6.96527 - 1351.0/(217.0 + t/°C); \text{ temp range 29–155°C} \] (Antoine eq. for liquid state, Dreisbach 1961)

3088 (calculated-Antoine eq., Weast 1972–73)

\[ \log (P/\text{mmHg}) = [-0.2185 \times 9163.2/(T/K)] + 8.079996; \text{ temp range –24 to 113.9°C} \] (Antoine eq., Weast 1972–73)

2910 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

\[ \log (P/\text{mmHg}) = 6.95185 - 1314.41/(209.197 + t/°C); \text{ temp range 49.97–113.7°C} \] (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)

3218 (calculated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P/\text{mmHg}) = 6.95185 - 1314.41/(209.20 + t/°C); \text{ temp range 50–114°C} \] (Antoine eq., Dean 1985, 1992)

92.1 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Moukerjee 1975)

94.2 (calculated-P/C, Dilling 1977)

78.4 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

122, 120 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)

81.4* (24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)

92.2* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

\[ \ln [\text{H/(atm·m}^3/\text{mol})] = 9.320 - 4943/(T/K); \text{ temp range 10–30°C} \] (EPICS measurements, Ashworth et al. 1988)

74.97 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

97.34 (computed value, Yaws et al. 1991)

70.9, 115.5, 172.3 (20, 30, 40°C, infinite dilution activity coeff. \(\gamma\)-GC, Tse et al. 1992)

67.1, 136, 234 (20, 35, 50°C, activity coeff \(\gamma\)-differential pressure transducer, Wright et al. 1992)

82* (26.2°C, EPICS-GC, measured range 26.2–44.8°C, Hansen et al. 1993)

\[ \ln [\text{H/(kPa·m}^3/\text{mol})] = -5091/(T/K) + 17.0; \text{ temp range 26.2–45°C} \] (EPICS-GC measurements, Hansen et al. 1993)
1.30, 2.48 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)


66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)

65.7 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

66.78 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_\text{AW} = 5.219 – 1989/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{\text{OW}} at 25°C or as indicated. Additional data at other temperature designated * are compiled at the end of this section:

2.17 (calculated as per Tute 1971, Callahan et al. 1979; Ryan et al. 1988)

2.38 (Hansch & Leo 1979)

1.89 (shake flask, Log P Database, Hansch & Leo 1987)

1.89 (recommended, Sangster 1993)

2.07 (calculated-activity coefficients, Tse & Sandler 1994)

1.98* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)

1.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{\text{OA}} at 25°C:

3.40 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

< 1.0 (Kawasaki 1980; quoted, Howard 1990)

1.519 (microorganisms-water, calculated-K_{\text{OW}}, Mabey et al. 1982)

1.23 (quoted, Isnard & Lambert 1988)

1.049 (calculated-K_{\text{OW}}, McCarty et al. 1992)

Sorption Partition Coefficient, log K_{\text{OC}}:

1.845 (sandy soil column, Wilson et al. 1981)

1.748 (sediment-water, calculated-K_{\text{OW}}, Mabey et al. 1982)

3.20; 1.90 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

1.88 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constant, k, and Half-Lives, t_1/2:

Volatile: t_1/2 = 21 min, estimated from lab. experiment of initial 1 mg/L in water stirred at 200 rpm at 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Howard 1990)

Evaporation t_1/2(exptl) = 35.1 min, t_1/2(calc) = 6.1 min, 30.1 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{\text{OH}} for reaction with OH radical, k_{\text{NO3}} with NO3 radical and k_{\text{O3}} with O3, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{\text{OH}}* = (3.18 ± 0.06) × 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 295 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

k_{\text{OH}} = 3.3 × 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, with estimated residence time of 35 d, loss of 2.8% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k << 360 M^{-1} h^{-1} for singlet oxygen and k = 3.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation t_{1/2} ~ 196–1956 h, based on measured rate constants for reaction with hydroxyl radical in air (estimated, Atkinson 1985; quoted, Howard et al. 1991)

k_{\text{OH}}* = (3.18 ± 0.2) × 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 295 K, measured range 277–461 K (discharge flow-resonance fluorescence, Jeong et al. 1984)

k_{\text{OH(aq.)}} ≤ 0.08 M^{-1} \text{ s}^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with t_{1/2} ≥ 5 d at pH 7 (Yao & Haag 1991).

k_{\text{OH(aq.)}} = 1.1 × 10^{8} \text{ M}^{-1} \text{ h}^{-1} for the reaction with OH radical in aqueous solution (Haag & Yao 1992)
Hydrolysis:

\[ k = 1.2 \times 10^{-7} \, \text{h}^{-1} \] at 25°C and pH 7 (estimated, Mabey et al. 1982)

\[ k = 5.9 \times 10^{-3} \, \text{M}^{-1} \, \text{s}^{-1} \] with \( t_{1/2} = 3263 \, \text{h} \), based on alkaline catalyzed hydrolysis reaction at pH 9 and 25°C;

\( t_{1/2} = 37 \, \text{yr} \), based on hydrolysis rate constant measured at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard 1990; Howard et al. 1991)

\( t_{1/2} \) (abiotic) or \( t_{1/2} \) (dehydrohalogenation) = 170 months (Olsen & Davis 1990)

\[ t_{1/2} = 14000 \, \text{d} \] at pH 7, \( t_{1/2} = 0.14 \, \text{d} \) at pH 12 in natural waters (Capel & Larson 1905)

Biodegradation:

\[ t_{1/2} \] (aq. aerobic) = 4320–8760 h, based on the extremely low or no biodegradation which was observed in screening tests and a river die-away test (Tabak et al. 1981; Kawasaki 1980; Mudder & Musterman 1982; quoted, Howard 1990; Howard et al. 1991)

\[ t_{1/2} \] (aq. anaerobic) = 17280–35040 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991)

\[ k = 0.04 \, \text{yr}^{-1} \] with \( t_{1/2} = 24 \, \text{d} \) (Wood et al. 1985; quoted, Olsen & Davis 1990)

\[ t_{1/2} \] (aerobic) = 180 d, \( t_{1/2} \) (anaerobic) = 720 d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant \( k = 3 \times 10^{-12} \, \text{mL cell}^{-1} \, \text{h}^{-1} \) for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

\[ k_1 = 0.763 \, \text{h}^{-1} \] (flagfish, calculated-BCF \times k_2, McCarty et al. 1992)

\[ k_2 = 0.0676 \, \text{h}^{-1} \] (flagfish, estimated from one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance \( t_{1/2} = 2.4–24 \, \text{h} \) for the reaction with OH radical in air (Darnall et al. 1976);

photodecomposition \( t_{1/2} = 15.9 \, \text{h} \) with NO under simulated atmospheric conditions (Dilling et al. 1976);

estimated residence time of 35 d, loss of 2.8% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

\( t_{1/2} = 196–1956 \, \text{h} \), based on measured rate constants for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: estimated \( t_{1/2} = 1.9 \, \text{d} \) in surface waters in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

\( t_{1/2} = 3263–8760 \, \text{h} \), based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous degradation half-life (Howard et al. 1991)

Biodegradation \( t_{1/2} \) (aerobic) = 100 d, \( t_{1/2} \) (anaerobic) = 400 d and hydrolysis \( t_{1/2} = 14000 \, \text{d} \) at pH 7, \( t_{1/2} = 0.14 \, \text{d} \) at pH 12 in natural waters (Capel & Larson 1995)

\[ k(\text{exptl}) \leq 0.08 \, \text{M}^{-1} \, \text{s}^{-1} \] for direct reaction with ozone in water at pH 2 and 22°C, with \( t_{1/2} \geq 5 \, \text{d} \) at pH 7 (Yao & Haag 1991).

Ground water: \( t_{1/2} = 3263–117520 \, \text{h} \), based on estimated hydrolysis half-life pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and data from estimated unacclimated aerobic aqueous biodegradation half-life as well as a ground water die-away study in which no biodegradation was observed (Wilson et al. 1984; quoted, Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} = 3263–8760 \, \text{h} \), based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991) and a soil column test in which no biodegradation was observed (Wilson et al. 1981; quoted, Howard et al. 1991).

Biota:
TABLE 5.1.1.9.1
Reported aqueous solubilities of 1,1,2-trichloroethane at various temperatures

\[
S/(\text{wt%}) = 0.48137 - 2.9594 \times 10^{-3}(t/\degree C) + 4.3162 \times 10^{-5}(t/\degree C)^2 + 3.2190 \times 10^{-7}(t/\degree C)^3 \tag{1}
\]

\[
S/(\text{wt%}) = 2.89796 - 1.8585 \times 10^{-2}(T/\text{K}) + 3.48961 \times 10^{-5}(T/\text{K})^2 \tag{2}
\]

1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask</td>
<td>summary of literature data</td>
<td>activity coefficient</td>
<td></td>
</tr>
<tr>
<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
</tr>
<tr>
<td>0</td>
<td>4660</td>
<td>10</td>
<td>4600</td>
</tr>
<tr>
<td>20</td>
<td>4360</td>
<td>20</td>
<td>4410</td>
</tr>
<tr>
<td>25</td>
<td>4580</td>
<td>25</td>
<td>4380</td>
</tr>
<tr>
<td>55</td>
<td>5320</td>
<td>30</td>
<td>4390</td>
</tr>
<tr>
<td>40</td>
<td>4530</td>
<td>40</td>
<td>4830</td>
</tr>
<tr>
<td>60</td>
<td>5290</td>
<td>50</td>
<td>5950</td>
</tr>
<tr>
<td>70</td>
<td>6860</td>
<td>70</td>
<td>6961</td>
</tr>
<tr>
<td>eq. 1</td>
<td>( S/\text{wt%} )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>Stephenson 1992</th>
<th>Tse et al. 1992</th>
<th>Wright et al. 1992</th>
<th>Horvath &amp; Getzen 1999a</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC</td>
<td>activity coefficient</td>
<td>activity coefficient</td>
<td>tentative, IUPAC-NIST</td>
</tr>
<tr>
<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
</tr>
<tr>
<td>0</td>
<td>4640</td>
<td>20</td>
<td>4813</td>
</tr>
<tr>
<td>9.2</td>
<td>4390</td>
<td>30</td>
<td>5035</td>
</tr>
<tr>
<td>31.3</td>
<td>4580</td>
<td>40</td>
<td>5205</td>
</tr>
<tr>
<td>41</td>
<td>4830</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50.6</td>
<td>5180</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60.5</td>
<td>4970</td>
<td></td>
<td></td>
</tr>
<tr>
<td>710</td>
<td>5550</td>
<td></td>
<td></td>
</tr>
<tr>
<td>81.7</td>
<td>6380</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90.8</td>
<td>7030</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 2</td>
<td>( S/\text{wt%} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>temp range</td>
<td>263–328 K</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.9.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.2
Reported vapor pressures of 1,1,2-trichloroethane at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ebulliometry</td>
<td></td>
<td>summary of literature data</td>
<td></td>
<td>ebulliometry</td>
</tr>
<tr>
<td>73.5</td>
<td>26664</td>
<td>-24.0</td>
<td>133.3</td>
<td>49.97</td>
<td></td>
</tr>
<tr>
<td>80.3</td>
<td>34397</td>
<td>2.0</td>
<td>666.6</td>
<td>61.29</td>
<td></td>
</tr>
<tr>
<td>82.4</td>
<td>37064</td>
<td>8.3</td>
<td>1333</td>
<td>85.99</td>
<td></td>
</tr>
<tr>
<td>83.8</td>
<td>38530</td>
<td>21.6</td>
<td>2666</td>
<td>100.34</td>
<td></td>
</tr>
<tr>
<td>85.6</td>
<td>41597</td>
<td>35.2</td>
<td>5333</td>
<td>113.67</td>
<td></td>
</tr>
<tr>
<td>96.2</td>
<td>59328</td>
<td>44.0</td>
<td>7999</td>
<td>113.5</td>
<td></td>
</tr>
<tr>
<td>104.6</td>
<td>77594</td>
<td>55.7</td>
<td>13332</td>
<td>113.5</td>
<td></td>
</tr>
<tr>
<td>108.7</td>
<td>87326</td>
<td>73.3</td>
<td>26664</td>
<td>113.5</td>
<td></td>
</tr>
<tr>
<td>109.8</td>
<td>90393</td>
<td>93.0</td>
<td>53329</td>
<td>113.5</td>
<td></td>
</tr>
<tr>
<td>111.3</td>
<td>94392</td>
<td>113.9</td>
<td>101325</td>
<td>113.5</td>
<td></td>
</tr>
<tr>
<td>113.5</td>
<td>101325</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.3
Reported Henry’s law constants of 1,1,2-trichloroethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{(T/K)} \quad (1) \quad \log K_{AW} = A - \frac{B}{(T/K)} \quad (1a)
\]

\[
\ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{(T/K)} \quad (2) \quad \log \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{(T/K)} \quad (2a)
\]

\[
\ln \left( k_H/\text{atm} \right) = A - \frac{B}{(T/K)} \quad (3)
\]

\[
\ln \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] = A - \frac{B}{(T/K)} \quad (4) \quad \ln \left[ \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right] = A - \frac{B}{(T/K)} \quad (4a)
\]

\[
K_{AW} = A - B \cdot \frac{(T/K)}{2} \quad (5)
\]

Leighton & Calo 1981

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>30.4</td>
</tr>
<tr>
<td>7.0</td>
<td>38.23</td>
</tr>
<tr>
<td>12.9</td>
<td>49.08</td>
</tr>
<tr>
<td>18.0</td>
<td>62.27</td>
</tr>
<tr>
<td>19.5</td>
<td>61.35</td>
</tr>
<tr>
<td>24.3</td>
<td>81.36</td>
</tr>
<tr>
<td>26.1</td>
<td>88.4</td>
</tr>
</tbody>
</table>

Ashworth et al. 1988

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>39.52</td>
</tr>
<tr>
<td>15</td>
<td>63.83</td>
</tr>
<tr>
<td>20</td>
<td>74.98</td>
</tr>
<tr>
<td>25</td>
<td>92.21</td>
</tr>
<tr>
<td>30</td>
<td>134.76</td>
</tr>
</tbody>
</table>

Treybal et al. 1946

Dreisbach & Schrader 1949

Stull 1947

Dilling 1997

m.p. = -36.3 °C

b.p. = 113.8 °C

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>70.9</td>
</tr>
<tr>
<td>30</td>
<td>115.5</td>
</tr>
<tr>
<td>40</td>
<td>172.3</td>
</tr>
</tbody>
</table>

Tse et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>26.2</td>
<td>82</td>
</tr>
<tr>
<td>35.8</td>
<td>184</td>
</tr>
<tr>
<td>44.8</td>
<td>259</td>
</tr>
</tbody>
</table>

Hansen et al. 1993

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>67.1</td>
</tr>
<tr>
<td>35</td>
<td>136</td>
</tr>
<tr>
<td>50</td>
<td>234</td>
</tr>
</tbody>
</table>

Wright et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(kPa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>67.1</td>
</tr>
<tr>
<td>35</td>
<td>136</td>
</tr>
<tr>
<td>50</td>
<td>234</td>
</tr>
</tbody>
</table>

Activity coefficient

Leighton & Calo 1981

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>67.1</td>
</tr>
<tr>
<td>35</td>
<td>136</td>
</tr>
<tr>
<td>50</td>
<td>234</td>
</tr>
</tbody>
</table>

Ashworth et al. 1988

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>67.1</td>
</tr>
<tr>
<td>35</td>
<td>136</td>
</tr>
<tr>
<td>50</td>
<td>234</td>
</tr>
</tbody>
</table>

Equation 4

\[
A = 17 \pm 3.36
\]

\[
B = 5901 \pm 1158
\]
**FIGURE 5.1.1.9.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloroethane.

**TABLE 5.1.1.9.4**
Reported octanol-water partition coefficients of 1,1,2-trichloroethane at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>log $K_{OW}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.98</td>
</tr>
<tr>
<td>35</td>
<td>1.93</td>
</tr>
<tr>
<td>50</td>
<td>1.94</td>
</tr>
</tbody>
</table>

enthalpy of transfer

$\Delta H/(kJ \text{ mol}^{-1}) = -20.2$.

$log K_{OW} = A - \Delta H/2.303RT$

<table>
<thead>
<tr>
<th>$A$</th>
<th>$\Delta H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0195</td>
<td>-20.2</td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.9.4** Logarithm of $K_{OW}$ versus reciprocal temperature for 1,1,2-trichloroethane.
5.1.1.10 1,1,1,2-Tetrachloroethane

Common Name: 1,1,1,2-Tetrachloroethane
Synonym:
Chemical Name: 1,1,1,2-tetrachloroethane
CAS Registry No: 630-20-6
Molecular Formula: CH₂ClCCl₃
Molecular Weight: 167.849
Melting Point (°C):
-70.2 (Lide 2003)
Boiling Point (°C):
130.2 (Lide 2003)
Density (g/cm³ at 20°C):
1.5406 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.5328 (25°C, Dreisbach 1961)
1.4819 (Dean 1985)
Molar Volume (cm³/mol):
109.0 (20°C, calculated-density)
135.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
34.78, 42.18 (normal boiling point, 25°C, Dreisbach 1961)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1090* (20°C, shake flask, measured range 0–50°C, Van Arkel & Vles 1936)
1110 (Seidell 1940)
1100* (shake flask, temp range 10–80°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 16.165 + 0.0236·(T/K), temp range 283–353 K (Walraevens et al. 1974)
1100 (interpolation of literature values, Dilling 1977)
215, 200, 202 (3, 20, 34°C, shake flask-GC, Chio & Freed 1977)
1110* (summary of literature data, temp range 0–80°C, Horvath 1982)
1206, 1280, 1292, 1321 (20, 30, 35, 40°C, infinite dilution activity coeff. γ–GC, Tse et al. 1992)
1178, 1382, 1492, 1607(20, 30, 40°C, infinite dilution activity coeff. γ–UNIFAC, Tse et al. 1992)
1005, 1093, 1056 (20, 30, 40°C, activity coeff. γ–differential pressure transducer, Wright et al. 1992)
1070* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 2.17896 – 1.3966 × 10⁻³·(T/K) + 2.93282 × 10⁻⁵·(T/K)², temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1767* (Antoine eq. regression, temp range 58–200°C, Stull 1947)
8851* (59.31°C, ebulliometry, measured range 59.31–130.2°C, Dreisbach & Shrader 1949)
1578 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.97560 – 1410.7/(214.0 + t°C); temp range 43–174°C (Antoine eq. for liquid state, Dreisbach 1961)
1778 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9296.5/(T/K)] + 7.938042; temp range –16.3 to 130.5°C (Antoine eq., Weast 1972–73)
1604 (calculated-Antoine eq., Boublík et al. 1973, 1984)
log (P/mmHg) = 6.89875 – 1365.876/(209.744 + t/°C); temp range 59–130°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)

1853 (20°C, interpolation of literature values, Dilling 1977)

log (P/kPa) = 6.02534 – 1366.919/(209.861 + t/°C); temp range 59.31–130.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

1578 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.1005 – 1410.7/(–59.15 + T/K); temp range 316–417 K (Antoine eq., Stephenson & Malanowski 1987)

1201, 2120, 2765, 3575 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)

log (P/mmHg) = –1.0712 – 2.5074 × 10³/(T/K) + 6.1536·log (T/K) – 1.8763 × 10⁻²·(T/K) + 1.0462 × 10⁻⁵·(T/K)²; temp range 203–624 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

272.7 (calculated-P/C, Dilling 1977)

283, 280 (calculated-P/C, recommended, Mackay & Shiu 1981)

172.2, 284, 365, 486 (20, 30, 35, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)

196, 320, 560 (20, 30, 40°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)

0.496, 0.80 (30, 40°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Octanol/Water Partition Coefficient, log K Ow:

3.03 (calculated, Müller & Klein 1992)

2.62, 2.62 (30, 40°C, infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K OC:

Environmental Fate Rate Constant, k, and Half-Lives, t½:

Volatilization: t½ = 43 min for the evaporation from dilute aqueous solution (Dilling et al. 1975)

Evaporation t½(exptl) = 42.3 min, t½(calc) = 2.01 min, 48.8 min from water (Dilling 1977)

Photolysis:

Oxidation:

Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 as indicated, *data at other temperatures see reference:

kOH < 1.0 × 10⁻¹⁴ cm³ molecule⁻¹ s⁻¹, residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation t½ = 2236–22361 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: k = 1.2 M⁻¹ s⁻¹ for reaction at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991); k = 4320 M⁻¹ h⁻¹ for base reaction at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991); abiotic hydrolysis or dehydrohalogenation t½ = 384 months (Mabey et al. 1983; quoted, Olsen & Davis 1990).

Biodegradation: aqueous aerobic t½ = 672–4320 h, based on acclimated river die-away rate data for 1,1,2,2-tetrachloroethane (Mudder 1981; quoted, Howard et al. 1991), unacclimated sea water (Pearson & McConnell 1975; quoted, Howard et al. 1991) and sub-soil grab sample data for a ground water aquifer for 1,1,1-trichloroethane (Wilson et al. 1983; quoted, Howard et al. 1991); aqueous anaerobic t½ = 2688–17280 h, based on aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:
$t_{1/2} = 2236\text{--}22361 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with OH radical in air
(Atkinson 1987; quoted, Howard et al. 1991);
estimated tropospheric lifetime of 1.9 yr (Nimitz & Skaggs 1992).
Surface water: $t_{1/2} = 16\text{--}1604 \text{ h}$, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).
Ground water: $t_{1/2} = 16\text{--}1604 \text{ h}$, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).
Sediment:
Soil: $t_{1/2} = 16\text{--}1604 \text{ h}$, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

### Table 5.1.1.10.1
Reported aqueous solubilities of 1,1,1,2-tetrachloroethane at various temperatures

\[
S/\text{wt%} = 0.11968 - 7.87116 \times 10^{-4} \left(\frac{t}{\text{°C}}\right) + 1.42253 \times 10^{-5} \left(\frac{t}{\text{°C}}\right)^2 + 7.24354 \times 10^{-8} \left(\frac{t}{\text{°C}}\right)^3 \quad (1)
\]
\[
S/\text{wt%} = 2.17896 - 1.3966 \times 10^{-3} \left(\frac{t}{\text{K}}\right) + 2.93282 \times 10^{-5} \left(\frac{t}{\text{K}}\right)^2 \quad (2)
\]


<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1200</td>
<td>10</td>
<td>1130</td>
<td>0</td>
<td>1197</td>
<td>20</td>
<td>1206</td>
</tr>
<tr>
<td>20</td>
<td>1090</td>
<td>20</td>
<td>1100</td>
<td>10</td>
<td>1133</td>
<td>30</td>
<td>1280</td>
</tr>
<tr>
<td>35</td>
<td>1150</td>
<td>25</td>
<td>1100</td>
<td>20</td>
<td>1102</td>
<td>35</td>
<td>1292</td>
</tr>
<tr>
<td>50</td>
<td>1250</td>
<td>30</td>
<td>1110</td>
<td>25</td>
<td>1100</td>
<td>40</td>
<td>1321</td>
</tr>
<tr>
<td>40</td>
<td>1160</td>
<td>40</td>
<td>1160</td>
<td>30</td>
<td>1108</td>
<td>45</td>
<td>1170</td>
</tr>
<tr>
<td>50</td>
<td>1250</td>
<td>50</td>
<td>1250</td>
<td>40</td>
<td>1156</td>
<td>50</td>
<td>1249</td>
</tr>
<tr>
<td>60</td>
<td>1390</td>
<td>60</td>
<td>1390</td>
<td>50</td>
<td>1293</td>
<td>70</td>
<td>1393</td>
</tr>
<tr>
<td>70</td>
<td>1590</td>
<td>80</td>
<td>1850</td>
<td>60</td>
<td>1393</td>
<td>80</td>
<td>1848</td>
</tr>
<tr>
<td>80</td>
<td>1850</td>
<td>80</td>
<td>1850</td>
<td>80</td>
<td>1848</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

eq. 1 S/wt%

2. Wright et al. 1992 & Horvath & Getzen 1999a & recommended, IUPAC-NIST

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1005</td>
<td>0</td>
<td>1200</td>
<td>0</td>
<td>1200</td>
</tr>
<tr>
<td>30</td>
<td>1093</td>
<td>5</td>
<td>1150</td>
<td>5</td>
<td>1150</td>
</tr>
<tr>
<td>40</td>
<td>1056</td>
<td>10</td>
<td>1110</td>
<td>10</td>
<td>1110</td>
</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>1080</td>
<td>15</td>
<td>1080</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>1070</td>
<td>20</td>
<td>1070</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>1070</td>
<td>25</td>
<td>1070</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>1080</td>
<td>30</td>
<td>1080</td>
</tr>
<tr>
<td></td>
<td></td>
<td>35</td>
<td>1100</td>
<td>35</td>
<td>1100</td>
</tr>
<tr>
<td></td>
<td></td>
<td>40</td>
<td>1130</td>
<td>40</td>
<td>1130</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
<td>1170</td>
<td>45</td>
<td>1170</td>
</tr>
<tr>
<td></td>
<td></td>
<td>50</td>
<td>1230</td>
<td>50</td>
<td>1230</td>
</tr>
</tbody>
</table>

eq. 2 S/wt%
temp range 273–323 K
**Figure 5.1.1.10.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

**Table 5.1.1.10.2**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
<th>Octanol-Water Partition Coefficient (log K&lt;sub&gt;OW&lt;/sub&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-16.3</td>
<td>133.3</td>
<td>8851</td>
</tr>
<tr>
<td>7.40</td>
<td>666.6</td>
<td>10114</td>
</tr>
<tr>
<td>19.3</td>
<td>1333</td>
<td></td>
</tr>
<tr>
<td>32.1</td>
<td>2666</td>
<td>42066</td>
</tr>
<tr>
<td>46.7</td>
<td>5333</td>
<td>67881</td>
</tr>
<tr>
<td>56.0</td>
<td>7999</td>
<td></td>
</tr>
<tr>
<td>68.0</td>
<td>13332</td>
<td></td>
</tr>
<tr>
<td>87.2</td>
<td>26664</td>
<td></td>
</tr>
<tr>
<td>108.2</td>
<td>53329</td>
<td></td>
</tr>
<tr>
<td>130.5</td>
<td>101325</td>
<td></td>
</tr>
<tr>
<td>mp°C</td>
<td>-68.7</td>
<td></td>
</tr>
</tbody>
</table>

Vapor pressure equations:

1. \( \log P = A - \frac{B}{T/K} \)
2. \( \log P = A - \frac{B}{(C + t/°C)} \)
3. \( \log P = A - \frac{B}{(C + T/K)} \)
4. \( \log P = A - \frac{B}{T/K} - C \log (T/K) \)

Octanol-water partition coefficients:

- **Stull 1947**
- **Dreisbach & Shrader 1949**
- **Bhatia & Sandler 1995**

Enthalpy of transfer:

\( \Delta H/(kJ \cdot mol^{-1}) = -20.2 \)
**FIGURE 5.1.10.2** Logarithm of vapor pressure versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

**FIGURE 5.1.10.3** Logarithm of $K_{OW}$ versus reciprocal temperature for 1,1,1,2-tetrachloroethane.
5.1.1.11 1,1,2,2-Tetrachloroethane

Common Name: 1,1,2,2-Tetrachloroethane
Synonym: sym-tetrachloroethane, acetylene tetrachloride
Chemical Name: 1,1,2,2-tetrachloroethane
CAS Registry No: 79-34-5
Molecular Formula: C₂H₂Cl₄, CHCl₂CHCl₂
Molecular Weight: 167.849
Melting Point (°C):
-42.4 (Lide 2003)
Boiling Point (°C):
145.2 (Lide 2003)
Density (g/cm³ at 20°C):
1.5953 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
1.59449, 1.58666 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
105.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
135.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
44.89, 36.18 (25°C, at normal boiling point, Dreisbach 1961)
45.78, 38.65 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2857 (volumetric method, Wright & Schaffer 1932)
2880, 3360 (20, 55.6°C, Van Arkel & Vles 1936)
2850 (Seidell 1940)
2900 (data presented in graph, temp range 0–70°C, McGovern 1943)
2960* (shake flask-GC, measured range 10–80°C, Walraevens et al. 1974)
log [S/(mol/L)] = 2070/(T/K) – 16.316 + 0.0222·(T/K), temp range 283–353 K (Walraevens et al. 1974)
3790, 3220, 3210 (3, 20, 34°C, shake flask-GC, Chou & Freed 1977)
3000 (literature average, Dilling 1977)
3230 (shake flask-GC, Chou et al. 1979)
3041 (37°C, shake flask-GC, Sato & Nakijima 1979)
2880 (20°C, recommended, Sørensen & Arit 1979)
2970 (shake flask-LSC, Banerjee et al. 1980)
2960 (23.5°C, elution chromatography, Schwartz 1980)
3850* (20°C, elution chromatography, measured range 10–30°C, Schwarz & Miller 1980)
2985 (shake flask-LSC, Veith et al. 1980)
2962* (summary of literature data, temp range 0–80°C, Horvath 1982)
866.4 (calculated-UNIFAC activity coeff., Arbuckle 1983)
2915 (30°C, headspace-GC, McNally & Grob 1984)
2985 (calculated-UNIFAC activity coeff., Banerjee 1985)
2870 (20°C, selected, Riddick et al. 1986)
2355, 2695, 3008 (20, 35, 50°C, infinite dilution activity coeff. γ−GC, Barr & Newsham 1987)
2910* (20°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson 1992)
2481, 2503, 2917, 3008 (20, 30, 35, 40°C, infinite dilution activity coeff. γ−GC, Tse et al. 1992)
778, 918, 994, 1074 (20, 30, 35, 40°C, infinite dilution activity coeff. γ−UNIFAC, Tse et al. 1992)
2422, 3140, 2612 (20, 30, 40°C, activity coeff. γ-differential pressure transducer, Wright et al. 1992)
2570 (20°C, activity coeff. γ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
2830* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 4.87975 – 3.0937 × 10−5·(T/K) + 5.20513 × 10−5·(T/K)2, temp range 276–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
827* (static method, extrapolated, measured range 31.1–146.7°C, Nelson 1930)
log (P/mmHg) = 8.06938 – 2167.83/(T/K); temp range 31.1–146.7°C (static method, Nelson 1930)
850* (Antoine eq. regression, temp range 65–243.5°C, Stull 1947)
560* (Ramsay-Young method, measured range 25–130°C, Matthews et al. 1950)
793 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.98240 – 1465.1/(211.0 + t°C); temp range 55–191°C (Antoine eq. for liquid state, Dreisbach 1961)
851 (interpolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9917.1/(T/K)] + 8.072583; temp range 31.1–146°C (Antoine eq., Weast 1972–73)
582 (calculated-Antoine eq., Boublik et al. 1973)
log (P/kPa) = 6.63168 – 1228.062/(179.972 + t°C); temp range 25–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
867 (literature average, Dilling 1977)
585 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.77919 – 1240.857/(181.401 + t°C); temp range 25–130°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2133 (McNally & Grob 1984)
log (P/mmHg) = 6.6317 – 1228.1/(279.9 + t°C); temp range 25–130°C (Antoine eq., Dean 1985, 1992)
793 (selected, Riddick et al. 1986)
log (P/kPa) = 6.1295 – 1444.3/(205.1 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
793 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.1073 – 1465.1/(62.15 + T/K); temp range 328–464 K (Antoine eq-I, Stephenson & Malanowski 1987)
log (P/kPa) = 5.98931 – 1365.692/(76.476 + T/K); temp range 377–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)
440, 848, 1154, 2550(20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 56.2356 – 4.4615 × 106/(T/K) – 16.556·log (T/K) – 3.5724 × 10−10·(T/K)2; temp range 229–645 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
46.2 (exptl. 1/KAW (C/w/Cb), Hine & Mookerjee 1975)
47.1 (calculated-P/C, Dilling 1977)
35.38* (22.0°C, equilibrium cell-GC, measured range 11.0–27.2°C, Leighton & Calo 1981)
48.5, 48.0 (calculated-P/C, recommended, Mackay & Shiu 1981)
25.3* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m3/mol)] = 1.726 – 2810/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
38.5 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
33.45 (computed value, Yaws et al. 1991)
30.4, 50.7, 60.8, 91.2 (20, 30, 35, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
40.3, 57.06, 120 (20, 30, 40°C, activity coeff. γ-differential pressure transducer, Wright et al. 1992)
34.4 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
34.12 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log KAW = 2.493 – 1255/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kow:
2.56 (calculated as per Tute 1971, Callahan et al. 1979)
2.39 (shake flask-LSC, Banerjee et al. 1980)
Halogenated Aliphatic Hydrocarbons

2.39  (shake flask-LSC, Veith et al. 1980)
2.79, 2.84  (calculated-UNIFAC with octanol and water mutual solubility considered, calculated-UNIFAC with octanol and water mutual solubility not considered; Arbuckle 1983)
2.39  (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
2.93  (recommended, Sangster 1993)
2.39  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.9–1.0  (bluegill sunfish, Barrows et al. 1980; Kawasaki 1980)
0.90  (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
1.96  (microorganisms-water, calculated-KOC, Mabey et al. 1982)
0.91  (fathead minnow, Veith & Kosian 1982)
2.03  (calculated-KOC, McCarty et al. 1992)

Sorption Partition Coefficient, log KOC:

1.66  (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.90  (silt loam, quoted from Chiou et al. 1979; Karickhoff 1981; Howard 1990)
2.00, 1.80, 1.87  (estimated-KOC, estimated-S add mp, estimated-S, Karickhoff 1981)
2.07  (sediment-water, calculated-KOC, Mabey et al. 1982)
3.60  (soil, calculated-universal solvation model; Winget et al. 2000)

Sorption Partition Coefficient, log KOM:

1.66, 1.90  (quoted, calculated-MCI Z, Sabljic 1984)

Environmental Fate Rate Constant, k, and Half-Lives, t½:

Volatile: estimated experimental t½ = 56 min for initial concentration of 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation t½(exptl) = 55.2 min, t½(calc) = 12.0 min, 40.5 min from water (Dilling 1977); estimated t½ ~ 6.3 h for a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry’s law constant (Lyman et al. 1982; quoted, Howard 1990);

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:

k << 360 M–1 h–1 for singlet oxygen and k = 2.0 M–1 h–1 for peroxo radical at 25°C (Mabey et al. 1982)

kOH < 1.0 × 10–14 cm3 molecule–1 s–1, estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

k = 213–2131 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: k = 1.2 × 10–7 h–1 at 25°C and pH 7 (estimated, Mabey et al. 1982);

k0(abiotic) or k0(dehydrohalogenation) = 10 months (Mabey et al. 1983; quoted, Olsen & Davis 1990)

k0(abiotic) = 3.3 months (Cooper et al. 1987; quoted, Olsen & Davis 1990);

k = 2.3 × 107 M–1 yr–1 at pH 9 and 25°C with t½ = 1.1 d in alkaline soil, and k = 111 d at pH 7 (Kollig et al. 1987; quoted, Howard 1990)

k = 1.8 M–1 s–1 for base-catalyzed reaction at 25°C and pH 7 with t½ = 45 d;; k = 6480 M–1 h–1 for base reaction at pH 9 and 25°C; k = (27.6 ± 4.0) × 10–8 s–1 in sediment with 61% conversion (Haag & Mill 1988)

Biodegradation: k = (7.3 ± 0.1) × 10–3 min–1 with t½ = 6.6 d in sediment-water sample (Jafvert & Wolfe 1987)

k0(abiotic) > 800 d for the reaction with photochemically produced hydroxyl radical (Singh et al. 1981; quoted, Howard 1990)

k0(aq, aerobic) = 672–4320 h, based on acclimated river die-away rate data (Mudder 1981; quoted, Howard et al. 1991)
t½(aq. anaerobic) = 168–672 h, based on anaerobic sediment grab sample data (Jafvert & Wolfe 1987) and anaerobic screening test data (Hallen et al. 1986; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant of $3 \times 10^{-12}$ mL cell⁻¹ h⁻¹ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

$k_1 = 13.2$ h⁻¹ (flagfish, calculated-BCF \times k₂, McCarty et al. 1992)

$k_2 = 0.123$ h⁻¹ (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance $t_{vis} = 2.4–24$ h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{vis} = 213–2131$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: $t_{vis} = 6.6$ d in sediment-water sample (Jafvert & Wolfe 1987);

$t_{vis} = 45$ d at pH 7 and 25°C, based on based-catalyzed hydrolysis rate constant (Haag & Mill 1988);

$= 10.7–1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991);

Ground water: $t_{vis} = 10.7–1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Sediment: $t_{vis} = 6.6$ d in Bar-H sediment-water sample (Jafvert & Wolfe 1987);

measured $t_{vis} = 29$ d at 25°C, based on neutral and base-catalyzed hydrolysis rates studies in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: $t_{vis} < 10$ d (Ryan et al. 1988);

$= 10.7–1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Biota: $t_{vis} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$< 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

### TABLE 5.1.1.11.1

Reported aqueous solubilities of 1,1,2,2-tetrachloroethane at various temperatures

\[
\log S/(mol/L) = -15.316 + \frac{2070}{T/K} + B(T/K) \tag{1}
\]

\[
S/(wt\%) = 0.32934 - 2.10434 \times 10^{-3}(t/°C) + 2.54796 \times 10^{-5}(t/°C)^2 + 1.86126 \times 10^{-7}(t/°C)^3 \tag{2}
\]

\[
S/(wt\%) = 4.87975 - 3.0937 \times 10^{-3}(T/K) + 5.20513 \times 10^{-5}(T/K)^2 \tag{3}
\]

1.

<table>
<thead>
<tr>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
<th>T/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3200</td>
<td>10</td>
<td>3720</td>
<td>0</td>
<td>3299</td>
<td>20</td>
<td>2235</td>
</tr>
<tr>
<td>20</td>
<td>3010</td>
<td>20</td>
<td>3850</td>
<td>10</td>
<td>3116</td>
<td>35</td>
<td>2595</td>
</tr>
<tr>
<td>25</td>
<td>2960</td>
<td>30</td>
<td>3670</td>
<td>20</td>
<td>2995</td>
<td>50</td>
<td>3008</td>
</tr>
<tr>
<td>30</td>
<td>2940</td>
<td>30</td>
<td>3670</td>
<td>25</td>
<td>2962</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>2980</td>
<td>30</td>
<td>3670</td>
<td>30</td>
<td>2948</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>3120</td>
<td>40</td>
<td>2984</td>
<td>50</td>
<td>3118</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>3360</td>
<td>50</td>
<td>3356</td>
<td>70</td>
<td>3713</td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>3710</td>
<td></td>
<td></td>
<td>80</td>
<td>4199</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>4200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Eq. 1</th>
<th>S/(mol/L)</th>
<th>A</th>
<th>15.316</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.0222</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
2. Stephenson 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3170</td>
<td>0</td>
<td>3170</td>
<td>20</td>
<td>2481</td>
<td>20</td>
<td>2481</td>
</tr>
<tr>
<td>9.5</td>
<td>2900</td>
<td>30</td>
<td>2503</td>
<td>30</td>
<td>3140</td>
<td>40</td>
<td>2612</td>
</tr>
<tr>
<td>20</td>
<td>2910</td>
<td>35</td>
<td>2917</td>
<td>40</td>
<td>3008</td>
<td>15</td>
<td>2870</td>
</tr>
<tr>
<td>29.7</td>
<td>2920</td>
<td>40</td>
<td>3008</td>
<td>25</td>
<td>2840</td>
<td>25</td>
<td>2840</td>
</tr>
<tr>
<td>39.6</td>
<td>3010</td>
<td>50</td>
<td>2890</td>
<td>30</td>
<td>2830</td>
<td>40</td>
<td>2890</td>
</tr>
<tr>
<td>50.1</td>
<td>3160</td>
<td>35</td>
<td>2850</td>
<td>35</td>
<td>2850</td>
<td>45</td>
<td>3060</td>
</tr>
<tr>
<td>61</td>
<td>3570</td>
<td>40</td>
<td>2890</td>
<td>40</td>
<td>2890</td>
<td>50</td>
<td>3160</td>
</tr>
<tr>
<td>70.5</td>
<td>3850</td>
<td>45</td>
<td>3060</td>
<td>45</td>
<td>3060</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.6</td>
<td>4250</td>
<td>50</td>
<td>3160</td>
<td>50</td>
<td>3160</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stephenson 1992 shake flask-GC activity coefficient

1,1,2,2-Tetrachloroethane: solubility vs. 1/T

\[ \log x \text{ vs. } 1/T \]

**TABLE 5.1.11.1 (Continued)**

**FIGURE 5.1.11.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2,2-tetrachloroethane.
## TABLE 5.1.11.2
Reported vapor pressures of 1,1,2,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.1</td>
<td>1000</td>
<td>-3.80</td>
<td>133.3</td>
<td>25.0</td>
<td>560</td>
</tr>
<tr>
<td>34.6</td>
<td>1067</td>
<td>20.7</td>
<td>666.6</td>
<td>30.0</td>
<td>667</td>
</tr>
<tr>
<td>39.3</td>
<td>1533</td>
<td>33.0</td>
<td>1333</td>
<td>35.0</td>
<td>1080</td>
</tr>
<tr>
<td>44.3</td>
<td>2200</td>
<td>46.2</td>
<td>2666</td>
<td>40.0</td>
<td>1493</td>
</tr>
<tr>
<td>50.4</td>
<td>3120</td>
<td>60.8</td>
<td>5333</td>
<td>45.0</td>
<td>2000</td>
</tr>
<tr>
<td>57.8</td>
<td>4253</td>
<td>70.0</td>
<td>7999</td>
<td>50.0</td>
<td>2680</td>
</tr>
<tr>
<td>64.6</td>
<td>5893</td>
<td>83.2</td>
<td>13332</td>
<td>55.0</td>
<td>3480</td>
</tr>
<tr>
<td>72.3</td>
<td>8293</td>
<td>102.2</td>
<td>26664</td>
<td>60.0</td>
<td>4440</td>
</tr>
<tr>
<td>79.0</td>
<td>10879</td>
<td>124.0</td>
<td>53329</td>
<td>65.0</td>
<td>5626</td>
</tr>
<tr>
<td>85.0</td>
<td>13865</td>
<td>145.9</td>
<td>101325</td>
<td>70.0</td>
<td>6933</td>
</tr>
<tr>
<td>89.9</td>
<td>16785</td>
<td>75.0</td>
<td>8533</td>
<td></td>
<td></td>
</tr>
<tr>
<td>94.9</td>
<td>20438</td>
<td>mp/°C</td>
<td>-36</td>
<td>80.0</td>
<td>10666</td>
</tr>
<tr>
<td>99.9</td>
<td>24611</td>
<td>85.0</td>
<td>13066</td>
<td></td>
<td></td>
</tr>
<tr>
<td>105</td>
<td>29851</td>
<td>90.0</td>
<td>16079</td>
<td></td>
<td></td>
</tr>
<tr>
<td>109.1</td>
<td>34770</td>
<td>95.0</td>
<td>19532</td>
<td></td>
<td></td>
</tr>
<tr>
<td>114.9</td>
<td>41730</td>
<td>100</td>
<td>23665</td>
<td></td>
<td></td>
</tr>
<tr>
<td>119.9</td>
<td>47703</td>
<td>105</td>
<td>28331</td>
<td></td>
<td></td>
</tr>
<tr>
<td>120.1</td>
<td>48569</td>
<td>110</td>
<td>33130</td>
<td></td>
<td></td>
</tr>
<tr>
<td>124.5</td>
<td>54865</td>
<td>115</td>
<td>38930</td>
<td></td>
<td></td>
</tr>
<tr>
<td>130.4</td>
<td>66328</td>
<td>120</td>
<td>45663</td>
<td></td>
<td></td>
</tr>
<tr>
<td>135.2</td>
<td>92139</td>
<td>135</td>
<td>53329</td>
<td></td>
<td></td>
</tr>
<tr>
<td>141.5</td>
<td>102285</td>
<td>130</td>
<td>62795</td>
<td></td>
<td></td>
</tr>
<tr>
<td>146.7</td>
<td>106938</td>
<td>202</td>
<td>626.6*</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>626.6*</td>
<td>bp/K</td>
<td>420.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>826.6*</td>
<td>ΔHv = 38.42 kJ/mol at bp</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Kirchhoff, Rankine, Dupre eq.

<table>
<thead>
<tr>
<th>eq.</th>
<th>P/mmHg</th>
<th>eq.</th>
<th>P/mmHg</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>8.08938</td>
<td>A</td>
<td>35.117</td>
</tr>
<tr>
<td>B</td>
<td>2167.83</td>
<td>B</td>
<td>3646</td>
</tr>
<tr>
<td>C</td>
<td>8.981</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*extrapolated


**FIGURE 5.1.11.2** Logarithm of vapor pressure versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

**TABLE 5.1.1.11.3**

Reported Henry's law constants of 1,1,2,2-tetrachloroethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - \frac{B}{T/K} \quad (1) \\
\log K_{AW} = A - \frac{B}{T/K} \quad (1a) \\
\ln \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/K} \quad (2) \\
\log \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/K} \quad (2a) \\
\ln \left(\frac{1}{K_{AW}}\right) = A - \frac{B}{T/K} + C \cdot \left(\frac{1}{T/K}\right)^2 \quad (3) \\
\ln \left[\frac{1}{K_{AW}}\right] = A - \frac{B}{T/K} + C \cdot \left(\frac{1}{T/K}\right)^2 \quad (4) \\
\ln \left[\frac{1}{K_{AW}}\right] = A - \frac{B}{T/K} + C \cdot \left(\frac{1}{T/K}\right)^2 \quad (5)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>equilibrium cell-GC</strong></td>
<td><strong>EPICS-GC</strong></td>
<td><strong>activity coefficient</strong></td>
<td><strong>activity coefficient</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>11.0</td>
<td>19.95</td>
<td>10</td>
<td>33.44</td>
</tr>
<tr>
<td>13.0</td>
<td>22.83</td>
<td>15</td>
<td>20.27</td>
</tr>
<tr>
<td>21.0</td>
<td>31.06</td>
<td>20</td>
<td>73.97</td>
</tr>
<tr>
<td>22.0</td>
<td>35.38</td>
<td>25</td>
<td>25.33</td>
</tr>
<tr>
<td>27.2</td>
<td>38.19</td>
<td>30</td>
<td>70.93</td>
</tr>
<tr>
<td>eq. 3</td>
<td>H/atm</td>
<td>eq. 4a</td>
<td>H/(atm m³/mol)</td>
</tr>
<tr>
<td>A</td>
<td>14.91</td>
<td>A</td>
<td>1.726</td>
</tr>
<tr>
<td>B</td>
<td>3547</td>
<td>B</td>
<td>2810</td>
</tr>
</tbody>
</table>
**FIGURE 5.1.11.3** Logarithm of Henry’s law constant versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

1,1,2,2-Tetrachloroethane: Henry’s law constant vs. 1/T

Leighton & Calo 1981
Ashworth et al. 1988
Tse et al. 1992
Wright et al. 1992
Nicholson et al. 1994
Hovorka & Dohnal 1997

© 2006 by Taylor & Francis Group, LLC
5.1.1.12 Pentachloroethane

Common Name: Pentachloroethane
Synonym: 1,1,1,2,2-pentachloroethane, pentalin
Chemical Name: pentachloroethane
CAS Registry No: 76-01-7
Molecular Formula: C₂HCl₅, CHCl₂CCl₃
Molecular Weight: 202.294
Melting Point (°C):
–28.78 (Lide 2003)
Boiling Point (°C):
162.0 (Horvath 1982; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.6796 (Horvath 1982; Weast 1982–83)
1.6808, 1.6732 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
120 (calculated-density, Abernethy et al. 1988)
156.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
40.79, 36.941 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆H₅₆ (kJ/mol):
11.34 (Riddick et al. 1986)
Entropy of Fusion, ∆S₅₆ (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
345 (volumetric method, Wright & Schaffer 1932)
470 (20°C, shake flask, Van Arkel & Vles 1936)
463 (Seidell 1940)
500 (data presented in graph, temp range 0–70°C, McGovern 1943)
500* (shake flask-GC, temp range 10–80°C, Walraevens et al. 1974)
log [S/(mol dm–3)] = 2070/(T/K) – 16.412 + 0.0230·(T/K); temp range 283–353 K (Walraevens et al. 1974)
480 (literature average, Dilling et al. 1975; Dilling 1977)
776 (shake flask-LSC, Veith et al. 1980)
500* (summary of literature data, temp range 0–80°C, Horvath 1982)
500 (Dean 1985; Riddick et al. 1986)
470, 490 (20°C, 25°C, recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):
467* (25.1°C, static method, measured range 25.1–162.2°C, Nelson 1930)
log (P/mmHg) = 7.80304 – 2129.6/(T/K); temp range 25.1–162.2°C (static method, Nelson 1930)
596* (Antoine eq. regression, temp range 1.0–160.5°C, Stull 1947)
596 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9800.1/(T/K)] + 7.832202; temp range 1.0–160.6°C (Antoine eq., Weast 1972–73)
465 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.74011 – 1378.096/(197.367 + t°C); temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
600 (literature average, Dilling 1977)
453, 800 (20°C, 30°C, Verschueren 1983)
467  (calculated-Antoine eq., Boublik et al. 1984)
\[ \log (P/kPa) = 5.92765 - 1419.719/(202.285 + t/°C); \] temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
\[ \log (P/mmHg) = 6.740 - 1378/(197 + t/°C), \] temp range: 25–162°C (Antoine eq., Dean 1985, 1992)
590  (selected, Riddick et al. 1986)
\[ \log (P/kPa) = 5.7199 - 1295.67/(188.96 + t/°C); \] temp range not specified (Antoine eq., Riddick et al. 1986)
625  (calculated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 6.69025 - 1982.65/(–10.577 + T/K); \] temp range 274–434 K (Antoine eq., Stephenson & Malanowski 1987)
467, 453  (quoted, calculated-UNIFAC, Banerjee et al. 1990)
\[ \log (P/mmHg) = 72.1134 - 4.6522 \times 10^3/(T/K) - 23.777 \log (T/K) + 9.6908 \times 10^{-3}(T/K)^{-3.3886 \times 10^{-13}}(T/K)^2; \] temp range 244–665 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
247.9  (exptl -1/Kₜₚ = Cₚ/Cᵥ, Hine & Mookerjee 1975)
247.9  (calculated-P/C, Dilling 1977)
96.44  (calculated-QSAR, Nirmalakhandan & Speece 1988)
196.5  (calculated-P/C, Howard 1990)
188.9, 53.73 (quoted, calculated-bond contribution method, Meylan & Howard 1991)
183.9  (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:
2.89  (shake flask-LSC, Veith et al. 1980)
3.05  (HPLC-RT correlation, McDuffie 1981; quoted, Sangster 1993)
3.22  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.826  (bluegill sunfish, Barrows et al. 1980)
1.83  (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
1.78  (fathead minnow, Veith & Kosian 1982)

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constant, k and Half-Lives, t_{½}:
Volatileization: estimated experimental t_{½} = 48 min for 1 mg/L aqueous solution when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975)
\[ \text{Evaporation} t_{½}(\text{exptl}) = 46.5 \text{ min}, \quad t_{½}(\text{calc}) = 2.3 \text{ min}, \quad 32 \text{ min} \] from water (Dilling 1977)
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:
\[ k_{OH}(\text{calc}) = 1.93 \times 10^{-14} \text{ cm}³ \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{OH}(\text{exptl}) = 2.33 \times 10^{-13} \text{ cm}³ \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: disappearance t_{½} = 2.4–24 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);
estimated tropospheric lifetime of 0.58 h (Nimitz & Skaggs 1992).
Surface water:
Ground water:
Sediment:
Soil:
Biota: t_{½} < 1 d in tissues of bluegill sunfish (Barrows et al. 1980).
### TABLE 5.1.12.1
Reported aqueous solubilities and vapor pressures of pentachloroethane at various temperatures

\[
\begin{align*}
S/(\text{wt%}) &= 5.41068 \times 10^{-2} - 2.81268 \times 10^{-4}(t/{^\circ}\text{C}) + 3.41333 \times 10^{-6}(t/{^\circ}\text{C})^2 + 4.76167 \times 10^{-8}(t/{^\circ}\text{C})^3 \quad (1) \\
\log S &= A/(T/\text{K}) - B + C(T/\text{K}) \quad (2)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Walraevans et al. 1974</strong></td>
<td><strong>Horvath 1982</strong></td>
</tr>
<tr>
<td>shake flask-GC</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>10</td>
<td>520</td>
</tr>
<tr>
<td>20</td>
<td>500</td>
</tr>
<tr>
<td>25</td>
<td>500</td>
</tr>
<tr>
<td>30</td>
<td>500</td>
</tr>
<tr>
<td>40</td>
<td>510</td>
</tr>
<tr>
<td>50</td>
<td>550</td>
</tr>
<tr>
<td>60</td>
<td>600</td>
</tr>
<tr>
<td>70</td>
<td>670</td>
</tr>
<tr>
<td>80</td>
<td>780</td>
</tr>
<tr>
<td>90</td>
<td>890</td>
</tr>
<tr>
<td>eq. 2</td>
<td>S/(mol/L)</td>
</tr>
<tr>
<td>A</td>
<td>2070</td>
</tr>
<tr>
<td>B</td>
<td>16.412</td>
</tr>
<tr>
<td>C</td>
<td>0.0230</td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>115.6</td>
</tr>
<tr>
<td>B</td>
<td>119.9</td>
</tr>
<tr>
<td>C</td>
<td>124.9</td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>128.7</td>
</tr>
<tr>
<td>B</td>
<td>132.4</td>
</tr>
<tr>
<td>C</td>
<td>134.6</td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>145.3</td>
</tr>
<tr>
<td>B</td>
<td>151.3</td>
</tr>
<tr>
<td>C</td>
<td>157.3</td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/Pa</td>
</tr>
</tbody>
</table>
**FIGURE 5.1.12.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for pentachloroethane.

**FIGURE 5.1.12.2** Logarithm of vapor pressure versus reciprocal temperature for pentachloroethane.
5.1.1.13 Hexachloroethane

Common Name: Hexachloroethane
Synonym: carbon hexachloride, perchloroethane, phenohep, HCE
Chemical Name: hexachloroethane
CAS Registry No: 67-72-1
Molecular Formula: C₂₇Cl₆, CCl₃CCl₃
Molecular Weight: 236.739
Melting Point (°C):
  186.8 (triple point) (Lide 2003)
Boiling Point (°C):
  184.7 (sublimation point) (Lide 2003)
Density (g/cm³ at 20°C):
  2.091 (McGovern 1943; Horvath 1982; Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
  113 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)
  177.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₚ (kJ/mol):
Entropy of Fusion, ΔSₚ (J/mol K):
Fugacity Ratio at 25°C, F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  50 (22.3°C, shake flask, Van Arkel & Vles 1936)
  50 (22.3°C, McGovern 1943)
  27.2 (shake flask-LSC, Veith et al. 1980)
  50 (22.3°C, recommended, Horvath 1982)
  77.1 (20°C, EPICS-LSC, Munz & Roberts 1986)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  42.7* (gas saturation method, extrapolated, measured range 31–55°C, Nelson 1930)
  75.4* (extrapolated-Antoine eq. regression, temp range 32.7–186.5°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 11711.3/(T/K)] + 8.440623; temp range 32.7–185.6°C (Antoine eq., Weast 1972–73)
  49.5 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 7.9015 – 3077/(T/K); temp range 317–345 K (Antoine eq.-II, solid, cubic, Stephenson & Malanowski 1987)
  7.856 – 2677/(T/K); temp range 345–460 K (Antoine eq.-I, solid, rhombic, Stephenson & Malanowski 1987)
  6.6075 – 2103.6/(T/K); temp range 460–513 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
  log (P/mmHg) = –366.2243 + 6.67893 × 10³/(T/K) + 155.63·log (T/K) – 0.15563·(T/K)²; temp range 306–698 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  231.3 (calculated as 1/Kₐw, Cₓ/Cₓ, reported as exp., Hine & Mookerjee 1975)
  123.9 (calculated-P/C, Dilling 1977)
log Kₐw = 6.982 – 2320/(T/K), temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)
846* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

\[ \ln \frac{[H]}{(\text{atm} \cdot \text{m}^3/\text{mol})} = 3.744 - 2550/(T/\text{K}) \]; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

253.3 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

226.7 (computed value, Yaws et al. 1991)

285 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

\[ \log K_{\text{AW}} = 6.982 - 2320/(T/\text{K}) \] (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):

4.14 (20°C, shake flask-GC, both phases, Chiou et al. 1977)

3.82 (HPLC-\( k' \) correlation, Könemann et al. 1979)

3.93 (shake flask-LSC, Veith et al. 1980)

4.05 (RP-HPLC-RT correlation, Veith et al. 1980)

4.04 (HPLC-RT correlation, McDuffie 1981)

4.14 (recommended, Sangster 1993)

4.14 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \( \log K_{\text{oa}} \) at 25°C:

4.47 (calculated-\( S_{\text{oc}} \) and vapor pressure \( P \), Abraham et al. 2001)

Bioconcentration Factor, \( \log BCF \):

0.92–3.23 (calculated-\( K_{\text{ow}} \), Veith et al. 1979, 1980)

2.143 (bluegill sunfish, Barrows et al. 1980)

2.14 (bluegill sunfish, Veith et al. 1980)

3.83 (microorganisms-water, calculated-\( K_{\text{ow}} \), Mabey et al. 1982)

2.14 (bluegill sunfish, Veith & Kosian 1982)

2.85 (fathead minnow, Veith & Kosian 1982)

4.57 (calculated-\( K_{\text{ow}} \), Thomann 1989)

Sorption Partition Coefficient, \( \log K_{\text{oc}} \):

4.3 (sediment-water, calculated-\( K_{\text{ow}} \), Mabey et al. 1982)

Environmental Fate Rate Constant, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization: estimated experimental \( t_{1/2} = 40–45 \) min from dilute aqueous solution in open container of depth 65mm and stirring at 200 rpm (Dilling et al. 1975)

Evaporation \( t_{1/2}(\text{exptl}) = 28.0 \) min, \( t_{1/2}(\text{calc}) = 4.5 \) min, 24.5 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO3}} \) with \( \text{NO}_3 \) radical and \( k_{\text{O3}} \) with \( \text{O}_3 \) or as indicated, *data at other temperatures see reference:

\( k_{\text{OH}} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), estimated residence time > 11600 d, loss = 0.0% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

\( t_{1/2} > 7.3–73 \) yr, based on estimated maximum rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not significant, based on hydrolysis studies after 13 d at 85°C and pH 3, 7, and 11 (Ellington et al. 1987; quoted, Howard et al. 1991)

\( t_{1/2}(\text{aq. aerobic}) = 672 \) h–4320 h, based on aqueous screening studies (Howard et al. 1991)

\( t_{1/2}(\text{aq. anaerobic}) = 2688–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

\( t_{1/2}(\text{aerobic}) = 28 \) d, \( t_{1/2}(\text{anaerobic}) = 110 \) d in natural waters (Capel & Larson 1995)

Biodegradation:

\( k = (5.0 \pm 0.34) \times 10^{-2} \text{ min}^{-1} \) in Bar-H sediment-water slurry, \( k = (2.0 \pm 0.17) \times 10^{-2} \text{ min}^{-1} \) in Beaver Dam sediment-water slurry, \( k = (2.6 \pm 0.2) \times 10^{-2} \text{ min}^{-1} \) in Hickory Hill sediment-water slurry, \( k = (1.9 \pm 0.16) \times 10^{-2} \text{ min}^{-1} \) in Memorial Park sediment-water slurry and \( k = (1.9 \pm 0.1) \times 10^{-2} \text{ min}^{-1} \) with \( t_{1/2} = 36 \) min in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

\( t_{1/2}(\text{aq. aerobic}) = 672 \) h–4320 h, based on aqueous screening studies (Howard et al. 1991)

\( t_{1/2}(\text{aq. anaerobic}) = 2688–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

\( t_{1/2}(\text{aerobic}) = 28 \) d, \( t_{1/2}(\text{anaerobic}) = 110 \) d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of \( 1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1} \) for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (\( k_{1} \)) and Elimination (\( k_{2} \)) Rate Constants or Half-Lives:
Halogenated Aliphatic Hydrocarbons

Half-Lives in the Environment:
Air: disappearance $t_{1/2} > 10$ d for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
$t_{1/2} > 7.3–73$ yr, based on estimated maximum rate constant for reaction with hydroxyl radical (Singh et al. 1980; quoted, Howard et al. 1991);
residence time $> 11600$ d, loss $= 0.0$ in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical K for the reaction with OH radical (Singh et al. 1981)
Surface water: $t_{1/2} = 36$ min in anoxic sediment-water suspension (Jafvert & Wolfe 1987);
$t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Residence time $> 11600$ d, loss $= 0.0$ in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical K for the reaction with OH radical (Singh et al. 1981)
Surface water: $t_{1/2} = 36$ min in anoxic sediment-water suspension (Jafvert & Wolfe 1987);
$t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Ground water: $t_{1/2} = 1344–8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment: disappearance $k = (5.0 \pm 0.34) \times 10^{-2}$ min$^{-1}$ in Bar-H sediment-water slurry, $k = (2.0 \pm 0.17) \times 10^{-2}$ min$^{-1}$ in Beaver Dam sediment-water slurry, $k = (2.6 \pm 0.2) \times 10^{-2}$ min$^{-1}$ in Hickory Hill sediment-water slurry, $k = (1.9 \pm 0.16) \times 10^{-2}$ min$^{-1}$ in Memorial Park sediment-water slurry and $k = (1.9 \pm 0.1) \times 10^{-2}$ min$^{-1}$ with $t_{1/2} = 36$ min in Bar-H sediment-water suspension (Jafvert & Wolfe 1987)
Soil: $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980)

<table>
<thead>
<tr>
<th>TABLE 5.1.1.13.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures and Henry’s law constant of hexachloroethane at various temperatures</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nelson 1930</td>
<td>Stull 1947</td>
</tr>
<tr>
<td>gas saturation</td>
<td>summary of literature data</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>$t/°C$</th>
<th>H/(Pa m$^3$/mol)</th>
<th>$t/°C$</th>
<th>H/(Pa m$^3$/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>31</td>
<td>73.3</td>
<td>32.7</td>
<td>133.3</td>
<td>10</td>
<td>601</td>
<td>10</td>
<td>74.2</td>
</tr>
<tr>
<td>35</td>
<td>93.3</td>
<td>49.8</td>
<td>666.6</td>
<td>15</td>
<td>566.4</td>
<td>20</td>
<td>285</td>
</tr>
<tr>
<td>40</td>
<td>133.3</td>
<td>73.5</td>
<td>1333</td>
<td>20</td>
<td>598.8</td>
<td>25</td>
<td>30</td>
</tr>
<tr>
<td>45</td>
<td>198.7</td>
<td>87.6</td>
<td>2666</td>
<td>30</td>
<td>1044</td>
<td>25</td>
<td>846.1</td>
</tr>
<tr>
<td>50</td>
<td>282.6</td>
<td>102.3</td>
<td>5333</td>
<td>30</td>
<td>1044</td>
<td>30</td>
<td>537</td>
</tr>
<tr>
<td>55</td>
<td>390.6</td>
<td>112.0</td>
<td>7999</td>
<td>124.2</td>
<td>13332</td>
<td>143.1</td>
<td>26664</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>ln [H/(atm·m$^3$/mol)] = A – B/(T/K)</td>
<td>163.8</td>
<td>53332</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>A = 3.744</td>
<td></td>
<td>B = 2550</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>185.6</td>
<td>101325</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
5.1.1.14 1-Chloropropane (n-Propyl chloride)

Common Name: 1-Chloropropane
Synonym: n-Propyl chloride, propyl chloride
Chemical Name: 1-chloropropane, n-Propyl chloride, propyl chloride
CAS Registry No: 540-54-5
Molecular Formula: CH₃CH₂CH₂Cl
Molecular Weight: 78.541
Melting Point (°C):
46.5  (Lide 2003)
Boiling Point (°C):
46.5*  (Lide 2003)
Density (g/cm³ at 20°C):
0.8909  (Dreisbach 1961; Horvath 1982)
0.8899, 0.8830  (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
88.3  (20°C, calculated-density)
94.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
28.48, 27.25  (25°C, normal bp, Dreisbach 1961)
28.50, 27.24  (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
5.544  (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2720*  (20°C, measured range 0–30°C, volumetric method, Rex 1906)
2500  (Wright & Schaffer 1932)
2772  (30°C, shake flask, Van Arkel & Vles 1936)
2334  (Seidell 1941)
2333  (20°C, Saracco & Spaccamela Marchetti 1958)
2700  (20°C, Verschueren 1983)
2651*  (summary of literature data, Horvath 1982)
2710  (20°C, quoted, Riddick et al. 1986)
2500*  (reported value of IUPAC-NIST Solubility Data Series, temp range 0–37°C, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
37360, 55240  (20°C, 30°C, Rex 1906)
46500*  (interpolated-Antoine eq. regression, temp range –68.3 to 36.5°C, Stull 1947)
46000  (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.93111 – 1121.123/(230.2 + t°C); temp range –25 to 88°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.93111 – 1121.123/(230.2 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.93111 – 1121.123/(230.2 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. for liquid state, Dreisbach 1961)
40517*  (21.8°C, differential thermal analysis, measured range –25.1 to 47.1°C, Kemme & Kreps 1969)
log (P/mmHg) = [–0.2185 × 7485.7/(T/K)] + 8.028733; temp range –63.8 to 46.4°C (Antoine eq., Weast 1972–73)
log (P/kPa) = 6.07206 – 1120.381/(229.061 + t°C); temp range –25.1 to 47.1°C (Antoine eq. from reported explt. data of Kemme & Kreps 1969, Boublik et al. 1984)
log (P/mmHg) = 6.92648 – 1110.19/(227.94 + t°C); temp range –25 to 47°C (Antoine eq., Dean 1985, 1992)
Halogenated Aliphatic Hydrocarbons

45920 (selected, Riddick et al. 1986)
\[ \log (P/kPa) = 6.0765 - \frac{1125.09}{229.86 + t/°C}; \text{temp range not specified (Antoine eq., Riddick et al. 1986)} \]
46060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 6.09145 - \frac{1126.383}{-43.78 + T/K}; \text{temp range 248–320 K (Antoine eq., Stephenson & Malanowski 1987)} \]
\[ \log (P/mmHg) = 32.3325 - \frac{2.485 \times 10^3}{T/K} - 8.8052 \cdot \log (T/K) + 8.9119 \cdot 10^{-11} \cdot (T/K)^2; \text{temp range 150–503 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa m³/mol at 25°C):
1341 (calculated-P/C, using Hine & Mookerjee 1975 data)
1600 (calculated-QSAR, Nirmalakhandan & Speece 1988)
1091 (computed value, Yaws et al. 1991)
1450 \( \gamma^∞ \) from gas stripping-GC, Li et al. 1993

Octanol/Water Partition Coefficient, log K\text{OW}:
2.04 (shake flask, Log P Database, Hansch & Leo 1987)
2.04 (recommended, Sangster 1989)
2.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K\text{OA}:
2.24 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K\text{OC}:

Environmental Fate Rate Constants, k and Half-Lives, \( t_\text{1/2} \):

Half-Lives in the Environment:
Air: disappearance \( t_\text{1/2} = 2.4–24 \) h from air for the reaction with OH radical (Darnall et al. 1976).

**TABLE 5.1.1.14.1**

Reported aqueous solubilities of 1-chloropropane at various temperatures

\[ \begin{align*}
S/(\text{wt}%) &= 0.3746 - 0.007725 \cdot (t/°C) + 1.05001 \times 10^{-6} \cdot (t/°C)^2 + 1.14998 \times 10^{-6} \cdot (t/°C)^3 \quad (1)
\end{align*} \]

<table>
<thead>
<tr>
<th>Rex 1966</th>
<th>Horvath 1982</th>
<th>Horvath &amp; Getzen 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>volumetric method</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>reported, IUPAC-NIST</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>0</td>
<td>3760</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>3230</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>2720</td>
<td>20</td>
</tr>
<tr>
<td>30</td>
<td>2770</td>
<td>25</td>
</tr>
<tr>
<td>&amp;</td>
<td>30</td>
<td>2684</td>
</tr>
<tr>
<td>eq. 1</td>
<td>( S/\text{wt}% )</td>
<td>30</td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.14.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-chloropropane.

TABLE 5.1.1.14.2
Reported vapor pressures of 1-chloropropane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/Pa</th>
<th>T/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–63.8</td>
<td>133.3</td>
<td>–25.1</td>
<td>3840</td>
</tr>
<tr>
<td>–50.0</td>
<td>666.6</td>
<td>–19.6</td>
<td>5320</td>
</tr>
<tr>
<td>–41.0</td>
<td>1333</td>
<td>–13.7</td>
<td>7386</td>
</tr>
<tr>
<td>–31.0</td>
<td>2666</td>
<td>–6.90</td>
<td>10599</td>
</tr>
<tr>
<td>–19.5</td>
<td>5333</td>
<td>1.20</td>
<td>16065</td>
</tr>
<tr>
<td>–12.1</td>
<td>7999</td>
<td>12.1</td>
<td>26691</td>
</tr>
<tr>
<td>–2.50</td>
<td>13332</td>
<td>21.8</td>
<td>40517</td>
</tr>
<tr>
<td>12.1</td>
<td>26664</td>
<td>34.9</td>
<td>67194</td>
</tr>
<tr>
<td>29.4</td>
<td>53329</td>
<td>47.1</td>
<td>103458</td>
</tr>
<tr>
<td>46.4</td>
<td>101325</td>
<td>eq. 2</td>
<td>P/mmHg</td>
</tr>
</tbody>
</table>

mp/°C  | –117 |

Stull 1947 summary of literature data  Kemme & Kreps 1969 differential thermal analysis

© 2006 by Taylor & Francis Group, LLC
**FIGURE 5.1.14.2** Logarithm of vapor pressure versus reciprocal temperature for 1-chloropropane.
5.1.1.15 2-Chloropropane

Common Name: 2-Chloropropane
Synonym: isopropyl chloride
Chemical Name: 2-chloropropane, isopropyl chloride
CAS Registry No: 75-29-6
Molecular Formula: C₃H₇Cl, CH₃CHClCH₃
Molecular Weight: 78.541
Melting Point (°C):
  –117.18 (Lide 2003)
Boiling Point (°C):
  35.7 (Lide 2003)
Density (g/cm³ at 20°C):
  0.8626, 0.8560 (20°C, 25°C, Dreisbach 1959)
  0.8617, 0.8563 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm³/mol):
  91.2 (20°C, calculated from density)
  94.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
Enthalpy of Fusion, ∆Hₔ (kJ/mol):
  7.39 (calculated, Dreisbach 1959)
Entropy of Fusion, ∆Sₔ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  3050* (20°C, measured range 0–30°C, volumetric method, Rex 1906)
  3444 (shake flask, Fühner 1924)
  3056 (Seidell 1940)
  3000 (Seidell 1941)
  2950 (selected exptl., Horvath 1982)
  3400 (Dean 1985)
  3040* (20°C, tentative values, temp range 0–30°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  58050, 83940 (20°C, 30°C, Rex 1906)
  53329* (18.1°C, summary of literature data, temp range –78.8 to 36.5°C, Stull 1947)
  70580 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.96540 – 1081.6/(230 + t°C); temp range –32 to 90°C (Antoine eq. for liquid state, Dreisbach 1959)
  68700 (interpolated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.91997 – 1081.4/(232 + t°C); temp range –33 to 68°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 6855.2/(T/K)] + 7.75768; temp range –78.8 to 36.5°C (Antoine eq., Weast 1972–73)
  70000 (interpolated-Antoine eq., Boulik et al. 1984)
log (P/kPa) = 6.91429 – 1593.593/(289.355 + t°C); temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boulik et al. 1984)
  69440 (interpolated-Antoine eq., temp range 0–30°C, Dean 1985, 1992)
log (P/mmHg) = 7.771 – 1582.0/(288.0 + t°C); temp range 0–30°C (Antoine eq., Dean 1985, 1992)
Halogenated Aliphatic Hydrocarbons

log (P/kPa) = 5.3643 – 779.7/(196.5 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.54823 – 860.49/(-66.25 + T/K); temp range 239–310 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 115.1259 – 4.6278 × 10³/(T/K) – 42.197·log (T/K) + 2.526 × 10⁻²·(T/K) – 9.8906 × 10⁻¹⁴·(T/K)²; temp range 156–589 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
1652 (calculated-P/C, using Hine & Mookerjee 1975 data)
1248 (calculated-QSAR, Nirmalakhandan & Speece 1988)
1468 (computed value, Yaws et al. 1991)
1836 (γ∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
1.69 (calculated-π const., Hansch et al. 1968)
1.90 (shake flask, Log P Database, Hansch & Leo 1987)
1.90 (recommended, Sangster 1989)
1.90 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, t_{½}:

Hydrolysis: rate constant k = 2.12 × 10⁷ s⁻¹ with t_{½} = 38 d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance t_{½} = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).
Surface water: t_{½} = 38 d at 25°C and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

**TABLE 5.1.1.15.1**

Reported aqueous solubilities and vapor pressures of 2-chloropropane at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rex 1906</td>
<td>Horvath 1982</td>
</tr>
<tr>
<td>volumetric method</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>0</td>
<td>440</td>
</tr>
<tr>
<td>10</td>
<td>362</td>
</tr>
<tr>
<td>20</td>
<td>305</td>
</tr>
<tr>
<td>30</td>
<td>304</td>
</tr>
<tr>
<td>30</td>
<td>304</td>
</tr>
<tr>
<td>mp/°C</td>
<td>-117</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**FIGURE 5.1.1.15.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-chloropropane.

**FIGURE 5.1.1.15.2** Logarithm of vapor pressure versus reciprocal temperature for 2-chloropropane.
5.1.1.16 1,2-Dichloropropane

Common Name: 1,2-Dichloropropane
Synonym: propylene chloride, propylene dichloride, \(\alpha,\beta\)-propylene dichloride
Chemical Name: 1,2-dichloropropane
CAS Registry No: 78-87-5
Molecular Formula: \(\text{C}_3\text{H}_6\text{Cl}_2\), \(\text{CH}_3\text{CHClCH}_2\text{Cl}\)
Molecular Weight: 112.986
Melting Point (\(^\circ\)C):

\(-100.53\) (Lide 2003)

Boiling Point (\(^\circ\)C):

96.40 (McGovern 1943; Timmermans 1950; Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm\(^3\) at 20\(^\circ\)C):

1.1560 (Dreisbach 1959, 1961; Horvath 1982; Weast 1982–83; Riddick et al. 1986)
1.1494 (25\(^\circ\)C, Dreisbach 1959, 1961)

Molar Volume (cm\(^3\)/mol):

98, 115.8 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):

36.33, 30.5 (25\(^\circ\)C, normal bp, Dreisbach 1961)
36.40, 32.004 (25\(^\circ\)C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):

6.40 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):

Fugacity Ratio at 25\(^\circ\)C, \(F\): 1.0

Water Solubility (g/m\(^3\) or mg/L at 25\(^\circ\)C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2800 (shake flask-interferometer, Gross 1929; Stephen & Stephen 1963)
2773 (Seidell 1940)
2700 (20\(^\circ\)C, McGovern 1943)
2750 (measured by Dow Chemical, Dreisbach 1955–1961)
2096 (shake flask-GC, Jones et al. 1977/1978)
3520 (shake flask-GC, Chio et al. 1979)
2800* (summary of literature data, Horvath 1982)
2420 (headspace-GC, McNally & Grob 1983)
2070 (30\(^\circ\)C, headspace-GC, McNally & Grob 1984)
2600 (Dean 1985)
2740 (selected, Riddick et al. 1986; Howard 1990)
3000*, 2900 (20\(^\circ\)C, 29.7\(^\circ\)C, shake flask-GC/TC, measured range 0–90.4\(^\circ\)C, Stephenson 1992)
3005, 3129, 3261 (20, 30, 40\(^\circ\)C, infinite dilution activity coeff. \(\gamma\)-GC, Tse et al. 1992)
3287, 3706, 4152 (20, 30, 40\(^\circ\)C, infinite dilution activity coeff. \(\gamma\)-UNIFAC, Tse et al. 1992)
2683, 2717, 3003 (20, 30, 40\(^\circ\)C, activity coeff. \(\gamma\)-differential pressure transducer, Wright et al. 1992)
2650 (20\(^\circ\)C, limiting activity coeff. \(\gamma\) by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
2740* (recommended, temp range 278.15–313.15 K, IUPAC-NIST Series, Hovorka & Getzen 1999)
\(S/(\text{wt}%) = 3.3285 - 0.021464 \cdot (T/K) + 3.7632 \cdot 10^{-5} \cdot (T/K)^2\), temp range 275–313 K (Hovorka & Getzen 1999)

Vapor Pressure (Pa at 25\(^\circ\)C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7200* (isoteniscope method, measured range 15–99.7\(^\circ\)C, Nelson & Young 1933)
\(\log (P/\text{mmHg}) = 7.7085 - 1782.8/(T/K)\); temp range 15–100\(^\circ\)C (isoteniscope, Nelson & Young 1933)
6930 (McGovern 1943)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- **298** (calculated-1/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)
- **31.21, 2261** (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
- **280** (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)

\[
\ln \left( \frac{k_p}{\text{atm}} \right) = 19.60 - 4333/(T/K); \text{temp range:} 1.9–24.9°C \text{ (equilibrium cell-concn ratio, Leighton & Calo 1981)}
\]

- **286** (gas stripping-GC, Warner et al. 1987)
- **362** (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

\[
\ln [H/(\text{atm·m}^3/\text{mol})] = 9.843 - 4708/(T/K); \text{temp range} 10–30°C \text{ (EPICS measurements, Ashworth et al. 1988)}
\]

- **233** (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
- **150** (computed value, Yaws et al. 1991)
- **213, 324, 486** (20, 30, 40°C, infinite dilution activity coeff. γ−GC, Tse et al. 1992)
- **216, 347, 497** (20, 35, 50°C, activity coeff. γ−differential pressure transducer, Wright et al. 1992)
- **3.37, 5.93** (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

- **222** (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
- **226.8** (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
- **232** (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

\[
\log K_{AW} = 4.878 - 1730/(T/K); \text{temp range} 2–70°C \text{ (summary of literature data, Staudinger & Roberts 2001)}
\]

- **227.6** (EPICS-SPME, measured range 2–70°C, Görgényi et al. 2002)

\[
\ln K_{AW} = 9.49 - 3494.7/(T/K); \text{temp range} 2–70°C \text{ (EPICS-SPME method, Görgényi et al. 2002)}
\]

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- **2.00** (Hansch & Leo 1979)
- **1.98** (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
- **1.99** (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
Octanol/Air Partition Coefficient, $\log K_{OA}$:
- 2.96 (calculated-measured infinite dilution activity coeff. and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:
- < 1.0 (fish, Kawasaki 1980; quoted, Howard 1990)
- 1.29 (calculated-$K_{OC}$, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:
- 1.43 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
- 1.67 (silt loam soil, quoted from Chiou et al. 1979; Howard 1990)
- 1.70 (calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatile: $t_{1/2} < 50$ min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Mills et al. 1982);
- $t_{1/2} = 8$ min from a stirred solution 1.6 cm deep (Chiou et al. 1980; quoted, Howard 1990);
- $t_{1/2} = 1.7–10$ d, estimated from an EXAMS model of the fate of 1,2-dichloropropane in a pond, river, and two lakes (Burns 1981; quoted, Howard 1990);
- $t_{1/2} = 8.3$ h at 1 m depth of stirred aqueous solution (Lyman et al. 1982; quoted, Howard 1990);
- $t_{1/2} \approx 5.5$ h for the removal from a stream of 1 m depth with 1 m/s current, based on laboratory-determined relative transfer coefficients (Cadena et al. 1984; quoted, Howard 1990).

Photolysis:
- Oxidation, rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference: photooxidation $t_{1/2} = 65–646$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
- $k_{O_3(aq.)} \leq 0.004$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with a half-life of 100 d at pH 7 (Yao & Haag 1991).

Hydrolysis: $k = 5.0 \times 10^{-4}$ h$^{-1}$ at pH 7 to 9 and 25°C with a calculated $t_{1/2} = 15.8$ yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic $t_{1/2(aq.)} = 4008–30936$ h, based on acclimated aerobic soil grab sample data (Roberts & Stoydin 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2 (aq.)} = 16032–123744$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
- $t_{1/2} = 65–646$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $t_{1/2} > 23$ d, reaction with photochemically produced OH radical (Howard 1990).

Surface water: $t_{1/2} = 4008–30936$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); measured rate constant $k \leq 0.004$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 100$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 8016–61872$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Soil: $t_{1/2} = 4008–30936$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
### TABLE 5.1.1.16.1
Reported aqueous solubilities of 1,2-dichloropropane at various temperatures

\[
S/(\text{wt}%) = 0.1300 + 1.43332 \times 10^{-2 \cdot (t/°C)} - 4.99992 \times 10^{-4 \cdot (t/°C)^2} + 6.66654 \times 10^{-6 \cdot (t/°C)^3} \quad (1)
\]

\[
S/(\text{wt}%) = 3.3285 - 0.021464 \cdot (T/K) + 3.7632 \times 10^{-5 \cdot (T/K)^2} \quad (2)
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2300</td>
<td>20</td>
<td>2900</td>
<td>20</td>
<td>3005</td>
<td>5</td>
<td>2799</td>
</tr>
<tr>
<td>20</td>
<td>2700</td>
<td>9.5</td>
<td>2800</td>
<td>30</td>
<td>3129</td>
<td>10</td>
<td>2680</td>
</tr>
<tr>
<td>25</td>
<td>2800</td>
<td>29.7</td>
<td>2900</td>
<td>40</td>
<td>3261</td>
<td>15</td>
<td>268-</td>
</tr>
<tr>
<td>30</td>
<td>2900</td>
<td>40.3</td>
<td>3000</td>
<td>20</td>
<td>2700</td>
<td>25</td>
<td>2740</td>
</tr>
<tr>
<td>eq.1</td>
<td>S/wt%</td>
<td>49.8</td>
<td>3200</td>
<td>60</td>
<td>3500</td>
<td>35</td>
<td>2800</td>
</tr>
<tr>
<td></td>
<td></td>
<td>70.5</td>
<td>3900</td>
<td></td>
<td></td>
<td>40</td>
<td>2970</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80.2</td>
<td>4700</td>
<td>90.4</td>
<td>20</td>
<td></td>
<td>eq. 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2583</td>
<td>30</td>
<td></td>
<td>S/wt%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2717</td>
<td></td>
<td></td>
<td>temp range 275–313 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3003</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.16.1** Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for 1,1,2-trichloroethane.
TABLE 5.1.1.16.2
Reported vapor pressures of 1,2-dichloropropane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C\cdot\log(T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Nelson &amp; Young 1933</th>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>15.0</td>
<td>4400</td>
<td>-7.0</td>
<td>133.3</td>
</tr>
<tr>
<td>20.0</td>
<td>5600</td>
<td>17.3</td>
<td>666.6</td>
</tr>
<tr>
<td>25.0</td>
<td>7199</td>
<td>29.4</td>
<td>1333</td>
</tr>
<tr>
<td>30.0</td>
<td>8999</td>
<td>42.3</td>
<td>2666</td>
</tr>
<tr>
<td>35.0</td>
<td>11199</td>
<td>57.2</td>
<td>5333</td>
</tr>
<tr>
<td>40.0</td>
<td>13799</td>
<td>66.4</td>
<td>7999</td>
</tr>
<tr>
<td>45.0</td>
<td>16839</td>
<td>75.7</td>
<td>13332</td>
</tr>
<tr>
<td>50.0</td>
<td>20625</td>
<td>97.8</td>
<td>26664</td>
</tr>
<tr>
<td>55.0</td>
<td>24065</td>
<td>118.5</td>
<td>53329</td>
</tr>
<tr>
<td>60.0</td>
<td>30317</td>
<td>141.6</td>
<td>101325</td>
</tr>
<tr>
<td>65.0</td>
<td>36397</td>
<td></td>
<td></td>
</tr>
<tr>
<td>70.0</td>
<td>43570</td>
<td></td>
<td></td>
</tr>
<tr>
<td>75.0</td>
<td>51729</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.0</td>
<td>61235</td>
<td></td>
<td></td>
</tr>
<tr>
<td>85.0</td>
<td>71874</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90.0</td>
<td>84059</td>
<td></td>
<td></td>
</tr>
<tr>
<td>95.0</td>
<td>97792</td>
<td></td>
<td></td>
</tr>
<tr>
<td>96.0</td>
<td>100525</td>
<td></td>
<td></td>
</tr>
<tr>
<td>96.4</td>
<td>101325</td>
<td></td>
<td></td>
</tr>
<tr>
<td>99.7</td>
<td>112937</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloropropane.

© 2006 by Taylor & Francis Group, LLC
 Reported Henry’s law constants of 1,2-dichloropropane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \quad (1)
\]
\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2)
\]
\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)
\]
\[
\ln \left( H/(\text{Pa m}^3/\text{mol}) \right) = A - B/(T/K) \quad (4)
\]
\[
K_{AW} = A - B/(T/K) + C/(T/K)^2 \quad (5)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
</tr>
<tr>
<td>(1.90)</td>
<td>83.5</td>
<td>10</td>
<td>123.6</td>
</tr>
<tr>
<td>(13.5)</td>
<td>164.5</td>
<td>15</td>
<td>127.7</td>
</tr>
<tr>
<td>(15.7)</td>
<td>185.3</td>
<td>20</td>
<td>192.5</td>
</tr>
<tr>
<td>(17.1)</td>
<td>239.7</td>
<td>25</td>
<td>361.7</td>
</tr>
<tr>
<td>(22.0)</td>
<td>239.7</td>
<td>30</td>
<td>289.8</td>
</tr>
<tr>
<td>(24.9)</td>
<td>280.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[eq. 4\] \(H/(\text{atm m}^3/\text{mol})\)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
</tr>
<tr>
<td>(A)</td>
<td>19.6</td>
<td>(B)</td>
<td>4708</td>
</tr>
<tr>
<td>(B)</td>
<td>4333</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[eq. 3\] \(k_H/\text{atm}\)

\[eq. 1\] \(K_{AW}\)

**FIGURE 5.1.16.3** Logarithm of Henry’s law constant versus reciprocal temperature for 1,2-dichloropropane.
TABLE 5.1.16.4
Reported octanol-water partition coefficient of 1,2-dichloropropane at various temperatures

Bhatia & Sandler 1995

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.99</td>
</tr>
<tr>
<td>35</td>
<td>1.99</td>
</tr>
<tr>
<td>50</td>
<td>1.99</td>
</tr>
</tbody>
</table>

enthalpy of transfer

\[ \Delta H/(kJ \text{ mol}^{-1}) = -20.2 \]

log K_{OW} = A – \Delta H/2.303RT

A = 1.0195

\[ \Delta H = -20.2 \]

FIGURE 5.1.16.4 Logarithm of K_{OW} versus reciprocal temperature for 1,2-dichloropropane.
5.1.1.17 1,2,3-Trichloropropane

Common Name: 1,2,3-Trichloropropane
Synonym: 1,2,3-trichloropropane
Chemical Name: 1,2,3-trichloropropane
CAS Registry No: 96-18-4
Molecular Formula: 1,2,3-C₃H₅Cl₃, CH₂ClCHClCH₂Cl
Molecular Weight: 147.431
Melting Point (°C):
  -14.7 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
  157 (Lide 2003)
Density (g/cm³ at 20°C):
  1.3888 (Dreisbach 1961; Horvath 1982; Weast 1982–83)
  1.3832 (25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm³/mol):
  136.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  46.93, 37.12 (25°C, normal bp, Dreisbach 1961; Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  1900 (20°C, literature average, Dilling 1977)
  1896 (recommended, Horvath 1982)
  1900 (selected, Riddick et al. 1986)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  492 (extrapolated-Antoine eq., Dreisbach 1961)
  log (P/mmHg) = 6.98716 – 1502.3/(209.0 + t/°C); temp range 64–204°C (Antoine eq. for liquid state, Dreisbach 1961)
  log (P/mmHg) = [–0.2185 × 10714.3/(T/K)] + 8.326893; temp range 9.0–158°C (Antoine eq., Weast 1972–73)
  266.6, 533.2 (20°C, 30°C, Verschueren 1983)
  492.0 (calculated-Antoine eq., Stephenson & Malanowski 1987)
  log (P/kPa) = 6.11206– 1502.3/(–64.15 + T/K); temp range 337–477 K (Antoine eq., Stephenson & Malanowski 1987)
  413, 960 (quoted, calculated-solvatochromic parameters. and UNIFAC, Banerjee et al. 1990)
  log (P/mmHg) = -3.9501 – 2.4501 × 103/(T/K) + 6.6887·log (T/K) – 1.4991 × 10–2·(T/K) + 7.3403 × 10–6·(T/K)²;
  temp range 258–652 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section):
  32.22 (calculated-C/A/Cw, Dilling 1977)
  ln (kₛ/atm) = 14.61 – 3477/(T/K); temp range:1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
  24.91* (25.6°C, EPICS-GC, tap water, measured range 25.6–45°C, Tancréde & Yanagisawa 1990)
  log Kₛw = 3.351 – 1606/(T/K); temp range 26.5–45°C (EPICS measurements, Tancréde & Yanagisawa 1990)
  34.4 (computed value, Yaws et al. 1991)
  22.31 (interpolated from Tancréde & Yanagisawa 1990, Tancréde et al. 1992)
23.71 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
22.74 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
\[ \log K_{AW} = 3.073 - 1496/(T/K) \] (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 2.63 (estimated, Abernethy et al. 1988)
- 1.98 (quoted, Van Leeuwen et al. 1992; Verhaar et al. 1992)
- 2.25, 2.36 (quoted, calculated-molar volume, Wang et al. 1992)

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{OC} \):
- 1.98; 1.89; 1.92 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization: evaporation \( t_\frac{1}{2} = 51 \) min from dilute aqueous solution (Dilling 1975)
- Evaporation \( t_\frac{1}{2} \text{(exptl)} = 56.1 \) min, \( t_\frac{1}{2} \text{(calc)} = 18 \) min, 44.7 min from water (Dilling 1977)

Photolysis:
- Oxidation: photooxidation \( t_\frac{1}{2} = 61–613 \) h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- Hydrolysis: \( k = 1.8 \times 10^{-6} \) h\(^{-1} \) at pH 7 to 9 at 25°C with a calculated \( t_\frac{1}{2} = 44 \) yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation:
- Aerobic \( t_\frac{1}{2}(\text{aq.}) = 4320–8640 \) h, based on acclimated aerobic grab sample test data for 1,3-dichloropropane (Roberts & Stoydin 1976; quoted, Howard et al. 1991); anaerobic \( t_\frac{1}{2}(\text{aq.}) = 17280–34560 \) h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance \( t_\frac{1}{2} = 2.4–24 \) h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
- \( t_\frac{1}{2} = 61–613 \) h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: \( t_\frac{1}{2} = 4320–8640 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: \( t_\frac{1}{2} = 8640–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:
- Soil: disappearance \( t_\frac{1}{2} = 2.7 \) d was calculated from first-order kinetic for volatilization loss of mixtures in soils (Anderson et al. 1991);
- \( t_\frac{1}{2} = 4320–8640 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
TABLE 5.1.1.17.1
Reported Henry's law constants of 1,2,3-trichloropropane at various temperatures

Leighton & Calo 1981

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.90</td>
<td>21.27</td>
</tr>
<tr>
<td>13.5</td>
<td>20.90</td>
</tr>
<tr>
<td>15.7</td>
<td>24.71</td>
</tr>
<tr>
<td>17.1</td>
<td>25.86</td>
</tr>
<tr>
<td>22.0</td>
<td>27.58</td>
</tr>
<tr>
<td>24.9</td>
<td>36.13</td>
</tr>
</tbody>
</table>

\[ \ln (k_H/\text{atm}) = A - B/(T/\text{K}) \]

A 14.61
B 3477

FIGURE 5.1.1.17.1 Logarithm of Henry's law constant versus reciprocal temperature for 1,2,3-trichloropropane.
5.1.1.18 1-Chlorobutane (n-Butyl chloride)

Common Name: 1-Chlorobutane
Synonym: n-butyl chloride, butyl chloride
Chemical Name: 1-chlorobutane, n-butyl chloride
CAS Registry No: 109-69-3
Molecular Formula: C₄H₉Cl, CH₃CH₂CH₂CH₂Cl
Molecular Weight: 92.567
Melting Point (°C):
-123.1 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):
78.44 (Dreisbach 1959, 1961; Horvath 1982; Dean 1985)
78.4 (Lide 2003)

Density (g/cm³ at 20°C):
0.8862, 0.8808 (20°C, 25°C, Dreisbach 1959, 1961; Horvath 1982)
0.8857, 0.8810 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
117.1 (calculated-Le Bas method at normal boiling point)
104.5 (20°C, calculated-density)

Enthalpy of Vaporization, ∆HV (kJ/mol):
30.02, 33.32 (normal bp, 25°C, Dreisbach 1961)

Enthalpy of Fusion, ∆Hfus (kJ/mol):

Entropy of Fusion, ∆Sfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
666 (12.5°C, shake flask, Fühner 1924)
640 (Seidell 1940)
741 (Kakovsky 1957)
667 (17.5°C, Saracco & Spaccamela Marchetti 1958)
671 (20°C, exptl., Korenman et al. 1971; Horvath 1982)
614.7* (summary of literature data, Horvath 1982)
872 (generator column-HPLC, Tewari et al. 1982)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4173* (20°C, static method-manometer, measured range 20–70°C, Smyth & Engel 1929)
14170* (interpolated compiled data, temp range –49 to 77.8°C, Stull 1947)
13650 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.93790 – 1227.43/(224.1 + t°C); temp range 0–123°C (Antoine eq. for liquid state, Dreisbach 1959)
log (P/mmHg) = 6.93790 – 1227.433/(224.10 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
10639* (19.7°C, differential thermal analysis, measured range –16.7 to 78.5 °C, Kemme & Kreps 1969)
log (P/mmHg) = [–0.2185 × 8144.8/(T/K)] + 7.979366; temp range –49 to 77.8°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = 6.83694 – 1173.79/(218.13 + t°C), temp range: –17 to 78.6°C (Antoine eq., Dean 1985, 1992)
13300 (24.47°C, selected, Riddick et al. 1986)
log (P/kPa) = 6.0514 – 1216.82/(222.33 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
13660 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.0628 – 1227.433/(–49.05 + T/K); temp range 257–389 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 35.7808 – 2.8632 × 103/(T/K) –8.8957·log (T/K) + 5.1598 × 10–11·(T/K) + 3.5488 × 10–6·(T/K)²; temp range 150–537 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1800, 8600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

ln (kH/atm) = 18.51 – 3482/(T/K); temp range 1.0–23.0°C (equilibrium cell-conc ratio, Leighton & Calo 1981)

1708 (computed value, Yaws et al. 1991)

1878 (γ∞ from gas stripping-GC, Li et al. 1993)

1485 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

1384 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

Octanol/Water Partition Coefficient, log KOW:

2.39 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)
2.64 (shake flask, Hansch & Leo 1979; 1987)
2.55 (generator column-GC, DeVoe et al. 1981)
2.55 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
2.64 (recommended, Sangster 1989, 1993)
2.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KOA:

2.72 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, τ½:

Half-Lives in the Environment:

Air: disappearance t½ = 2.4–24 h from air for the reaction with OH radical (Darnall et al. 1976).

### TABLE 5.1.18.1
Reported aqueous solubilities and Henry’s law constants of 1-chlorobutane at various temperatures

\[
S/(wt\%) = 0.07703 - 6.75497 \times 10^{-4}(t/°C) - 1.00170 \times 10^{-10}(t/°C)^2 + 8.50030 \times 10^{-8}(t/°C)^3 \quad (1)
\]

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horvath 1982</td>
<td>Leighton &amp; Calo 1981</td>
</tr>
<tr>
<td>summary of literature data</td>
<td>equilibrium cell-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>0</td>
<td>770.3</td>
</tr>
<tr>
<td>10</td>
<td>703.6</td>
</tr>
<tr>
<td>20</td>
<td>642.0</td>
</tr>
<tr>
<td>25</td>
<td>614.7</td>
</tr>
<tr>
<td>30</td>
<td>590.6</td>
</tr>
</tbody>
</table>
### TABLE 5.1.1.18.1 (Continued)

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Horvath 1982</strong></td>
</tr>
<tr>
<td><strong>summary of literature data</strong></td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>eq. 1</td>
<td>S/wt%</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\ln (k_H/\text{atm}) = A - \frac{B}{T/\text{K}}
\]

\[
A = 18.51
\]

\[
B = 3482
\]

**FIGURE 5.1.1.18.1** Logarithm of mole fraction solubility (ln \(x\)) versus reciprocal temperature for 1-chlorobutane.

**FIGURE 5.1.1.18.2** Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorobutane.
TABLE 5.1.18.2
Reported vapor pressures of 1-chlorobutane at various temperatures and the coefficients for the vapor pressure equations

\[ \log P = A - B/(T/K) \] (1)  
\[ \log P = A - B/(C + t/°C) \] (2)  
\[ \log P = A - B/(C + T/K) \] (3)  
\[ \log P = A - B/(T/K) - C \log (T/K) \] (4)

<table>
<thead>
<tr>
<th>Method</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Smyth &amp; Engel 1929</strong></td>
<td>20.0</td>
<td>4173</td>
<td>–49.0</td>
<td>133.3</td>
<td>–16.7</td>
<td>1347</td>
<td>26.85</td>
<td>14719</td>
</tr>
<tr>
<td><strong>Stull 1947</strong></td>
<td>30.0</td>
<td>6799</td>
<td>–28.9</td>
<td>666.6</td>
<td>–10.5</td>
<td>2026</td>
<td>30.0</td>
<td>17001</td>
</tr>
<tr>
<td><strong>Kemme &amp; Kreps 1969</strong></td>
<td>40.0</td>
<td>10959</td>
<td>–18.6</td>
<td>1333</td>
<td>–6.20</td>
<td>2640</td>
<td>50.0</td>
<td>38434</td>
</tr>
<tr>
<td><strong>Gutsche &amp; Knapp 1982</strong></td>
<td>50.0</td>
<td>16892</td>
<td>–7.40</td>
<td>2666</td>
<td>0.80</td>
<td>3946</td>
<td>51.85</td>
<td>41397</td>
</tr>
<tr>
<td><strong>static-manometry</strong></td>
<td>60.0</td>
<td>25278</td>
<td>5.0</td>
<td>5333</td>
<td>6.20</td>
<td>5360</td>
<td>78.85</td>
<td>96925</td>
</tr>
<tr>
<td><strong>summary of literature data</strong></td>
<td>70.0</td>
<td>36170</td>
<td>13.0</td>
<td>7999</td>
<td>12.0</td>
<td>7306</td>
<td>80.0</td>
<td>106255</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–123.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*DTA—differential thermal analyzer

**FIGURE 5.1.18.3** Logarithm of vapor pressure versus reciprocal temperature for 1-chlorobutane.
5.1.1.19 2-Chlorobutane

Common Name: 2-Chlorobutane
Synonym: methylethylchloromethane, sec-butyl chloride
Chemical Name: 2-chlorobutane, methylethylchloromethane, sec-butyl chloride
CAS Registry No: 78-86-4
Molecular Formula: C₄H₉Cl, CH₃CH₂CHClCH₃
Molecular Weight: 92.567
Melting Point (°C):
  -131.3 (Dreisbach 1961; Horvath 1982; Lide 2003)
  -113.3, -140.5 (racemic, active, Riddick et al. 1986)
Boiling Point (°C):
  68.25 (Dreisbach 1961; Horvath 1982; Riddick et al. 1986)
  68.2 (Lide 2003)
Density (g/cm³ at 20°C):
  0.8732, 0.8677 (20°C, 25°C, Dreisbach 1961; Horvath 1982; Dean 1985)
  0.8732 (racemic, Riddick et al. 1986)
Molar Volume (cm³/mol):
  117.1 (calculated-Le Bas method at normal boiling point)
  106.0 (20°C, calculated-density)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
  31.81, 29.20 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
  1000 (volumetric method, Wright & Schaffer 1932)
  1000 (Dean 1985; Riddick et al. 1986)
  1070, 930, 850, 820, 840, 920 (0, 5, 10, 15, 20, 35°C, tentative values, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)
  \( S/(wt\%) = 8.9653 – 0.061598 \cdot (T/K) + 1.0678 \times 10^{-4} \cdot (T/K)^2 \), temp range 273–298 K (equation derived from reported solubility data, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  20210 (interpolated-Antoine eq., Dreisbach 1961)
  \[ \log (P/mmHg) = 6.94469 – 1195.8/(226.0 + t/°C); \text{temp range} -7 \text{to} 104°C \] (Antoine eq. for liquid state, Dreisbach 1961)
  \[ \log (P/mmHg) = [-0.2185 \times 7407.9/(T/K)] + 7.625620; \text{temp range} -60.2 \text{to} 68°C \] (Antoine eq., Weast 1972–73)
  \[ \log (P/mmHg) = 6.79923 – 1149.12/(224.68 + t/°C); \text{temp range} 0–40°C \] (Antoine eq., Dean 1985, 1992)
  \[ \log (P/mmHg) = 6.1222 – 1145.2/(234.4 + t/°C); \text{temp range not specified} \] (Antoine eq., Riddick et al. 1986)
  20200 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  \[ \log (P/kPa) = 6.06958 – 1195.8/(–47.15 + T/K); \text{temp range} 266–377 K \] (Antoine eq., Stephenson & Malanowski 1987)
  \[ \log (P/mmHg) = 28.2992 – 2.4355 \times 10^{11}/(T/K) – 7.359 \cdot \log (T/K) – 1.3048 \times 10^{-11} \cdot (T/K) + 3.0834 \times 10^{-6} \cdot (T/K)^2; \text{temp range} 142–521 K \] (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  2268* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)
  \[ \ln (k_H/\text{atm}) = 22.29 – 4499/(T/K); \text{temp range} 1.9–24.9°C \] (equilibrium cell-concn ratio, Leighton & Calo 1981)
Octanol/Water Partition Coefficient, log $K_{OW}$:
$$1.51$$
(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radicals (Darnall et al. 1976).

### TABLE 5.1.19.1
Reported Henry's law constants of 2-chlorobutane at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>$H/(Pa \cdot m^3/mol)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.90</td>
<td>653.3</td>
</tr>
<tr>
<td>13.5</td>
<td>1411</td>
</tr>
<tr>
<td>15.7</td>
<td>1545</td>
</tr>
<tr>
<td>17.1</td>
<td>1625</td>
</tr>
<tr>
<td>22.0</td>
<td>2023</td>
</tr>
<tr>
<td>24.9</td>
<td>2268</td>
</tr>
</tbody>
</table>

$\ln (k_H/atm) = A - B/(T/K)$

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>22.29</td>
</tr>
<tr>
<td>B</td>
<td>4499</td>
</tr>
</tbody>
</table>
5.1.1.20 1-Chloropentane (n-Amyl chloride)

Common Name: 1-Chloropentane
Synonym: n-amyl chloride, monochloropentane, pentyl chloride
Chemical Name: n-amyl chloride, 1-chloropentane, pentyl chloride
CAS Registry No: 543-59-9
Molecular Formula: C₅H₁₁Cl, CH₃CH₂CH₂CH₂CH₂Cl
Molecular Weight: 106.594
Melting Point (°C):
-99.0 (Dreisbach 1961; Horvath 1982; Riddick et al. 1982; Dean 1985; Lide 2003)
Boiling Point (°C):
108.4 (Lide 2003)
Density (g/cm³ at 20°C):
0.8818 (20°C, Weast 198–83; Horvath 1982)
0.8820, 0.8770 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
120.9 (20°C, calculated-density)
139.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
38.24, 32.77 (25°C, bp, Dreisbach 1961; Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
200 (volumetric method, Wright & Schaffer 1932)
789 (shake flask-residue volume method, Booth & Everson 1948)
190.6* (24.3°C, converted-distribution coeff., temp range 2.5–26.1°C, Leighton & Calo 1981)
198.2* (summary of literature data, Horvath 1982)
200 (Dean 1985; Riddick et al. 1986)
201* (tentative values, measured range 5–35°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)
S/(wt%) = 0.55726 – 3.7269 × 10⁻³·(T/K) + 6.457 × 10⁻⁶·(T/K)², temp range 276–310 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4142 (calculated-Antoine eq, Dreisbach 1961)
log (P/mmHg) = 6.96617 – 1332.890/(218.5 + t/°C); temp range 24–148°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.96617 – 1332.890/(218.50 + t/°C); pressure range 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
4142 (selected, Riddick et al. 1986)
log (P/kPa) = 5.93641 – 1271.15/(215.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
4148 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.09107 – 1332.89/(T/K – 54.65); temp range 289–409 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = -4.4886 – 2.2604 × 10⁻³(T/K) + 7.8088·log (T/K) – 2.3675 × 10⁻²·(T/K) + 1.4884 × 10⁻⁵·(T/K)²; temp range 174–568 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2209 (exptl.- 1/KₐW = Cₐ/W/Cₐ, Hine & Mookerjee 1975)
- 2480, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 2376* (24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)
  \( \ln (k_H/\text{atm}) = 23.04 - 4727/(T/K); \) temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
- 4942 (computed value, Yaws et al. 1991)
- 2407 (activity coefficient \( \gamma \) from gas stripping-GC, Li et al. 1993)
- 1835 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
  \( \log K_{AW} = 6.455 - 1928/(T/K) \) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 2.41 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{½} \):

Half-Lives in the Environment:

Air: disappearance \( t_\text{½} = 2.4–24 \text{ h} \) from air for the reaction with OH radical (Darnall et al. 1976).

### TABLE 5.1.1.20.1
Reported aqueous solubilities and Henry’s law constant of 1-chloropentane at various temperatures

\[
S/(\text{wt%}) = 0.02426 - 1.79166 \times 10^{-4} \cdot \text{(t/°C)} + 1.49999 \times 10^{-7} \cdot \text{(t/°C)}^2 - 3.33355 \times 10^{-9} \cdot \text{(t/°C)}^3 \quad (1)
\]

\[
S/(\text{wt%}) = 0.55726 - 3.7269 \times 10^{-3} \cdot \text{(T/K)} + 6.457 \times 10^{-6} \cdot \text{(T/K)}^2 \quad (2)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t'/°C )</td>
<td>converted-distribution coeff.</td>
<td>summary of literature data</td>
<td>summary of literature data</td>
<td>equilibrium cell-GC</td>
</tr>
<tr>
<td>S/g·m⁻³</td>
<td>S/g·m⁻³</td>
<td>S/g·m⁻³</td>
<td>S/g·m⁻³</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>2.5</td>
<td>200.6</td>
<td>0</td>
<td>242.6</td>
<td>5</td>
</tr>
<tr>
<td>7.0</td>
<td>205.2</td>
<td>10</td>
<td>224.8</td>
<td>10</td>
</tr>
<tr>
<td>12.9</td>
<td>196.8</td>
<td>20</td>
<td>207.1</td>
<td>15</td>
</tr>
<tr>
<td>18.0</td>
<td>195.0</td>
<td>25</td>
<td>198.2</td>
<td>20</td>
</tr>
<tr>
<td>19.5</td>
<td>200.5</td>
<td>30</td>
<td>189.3</td>
<td>25</td>
</tr>
<tr>
<td>24.3</td>
<td>190.6</td>
<td>35</td>
<td>209</td>
<td>30</td>
</tr>
<tr>
<td>26.1</td>
<td>203.2</td>
<td>eq. 1 S/wt%</td>
<td>eq. 2 S/wt%</td>
<td>eq. 2 S/wt%</td>
</tr>
<tr>
<td>2.5</td>
<td>661</td>
<td>( k_H/\text{atm} = A - B/(T/K) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0</td>
<td>846.6</td>
<td>A</td>
<td>23.04</td>
<td></td>
</tr>
<tr>
<td>12.9</td>
<td>1246</td>
<td>B</td>
<td>4727</td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.20.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for 1-chloropentane.

FIGURE 5.1.1.20.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chloropentane.
5.1.1.21 1-Chlorohexane

Common Name: 1-Chlorohexane
Synonym: n-hexyl chloride
Chemical Name: 1-chlorohexane
CAS Registry No: 544-10-5
Molecular Formula: C₆H₁₃Cl
Molecular Weight: 120.620
Melting Point (°C): –94 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C): 135.1 (Lide 2003)
Density (g/cm³):
0.8785; 0.8739 (20°C, 25°C, Dreisbach 1961)
0.8785 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
137.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
161.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
43.22, 35.39 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
83.6 (volumetric method, Wright & Schaffer 1932)
57.93* (23.0°C, converted-distribution coeff., temp range 1.0–23.0°C, Leighton & Calo 1981)
91.01* (summary of literature data, Horvath 1982)
54.3* (tentative values, measured range 5–25°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)
S/(wt%) = –0.019959 + 8.852 × 10⁻⁵·(T/K), temp range 274–296 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1284 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 7.0115 – 1437.05/(213.4 + t/°C); temp range 46–178°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 7.0115 – 1437.05/(213.4 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
1387* (26.7°C, differential thermal analysis, measured range 15–135.6°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.76886 – 1304.968/(t/°C + 200.058); temp range 15–135.6°C (Antoine eq. on exptl. data, Kemme & Kreps 1969)
1230 (interpolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.05136 – 1461.72/(t/°C + 136.92); temp range 15–136°C (Antoine eq. based on exptl. data of Kemme & Keeps 1969, Boublik et al. 1973)
1246 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.89376 – 1304.968/(T/K – 73.092); temp range: 288–409 K (Antoine eq., Stephenson & Malanowski 1987)
1260 (interpolated-Antoine eq., Dean 1992)
log (P/mmHg) = 7.05136 – 1461.72/(t/°C + 215.57); temp range 15–136°C (Antoine eq., Dean 1992)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2312* (23°C, equilibrium cell-concn ratio-GC/FID, measured range 1–23°C, Leighton & Calo 1981)

\[ \ln \left( \frac{K_H}{\text{atm}} \right) = 22.16 - \frac{4469}{(T/K)}; \text{temp range } 1.0-23.0°C \] (equilibrium cell-concn ratio, Leighton & Calo 1981)

1899 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

\[ \log K_{AW} = 6.073 - 1812/(T/K) \] (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

3.68 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \) or log \( K_B \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \) and Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:

---

**TABLE 5.1.1.21.1**

**Reported aqueous solubilities and Henry’s law constant of 1-chlorohexane at various temperatures**

\[ S/(\text{wt%}) = 0.01172 - 0.000313(t/°C) - 1.078 \times 10^{-5}(t/°C)^2 - 4.58 \times 10^{-7}(t/°C)^3 \] (1)

\[ S/(\text{wt%}) = -0.019959 + 8.852 \times 10^{-5}(T/K) \] (2)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>1.0</td>
<td>36.87</td>
<td>0</td>
<td>117.2</td>
<td>5</td>
</tr>
<tr>
<td>3.0</td>
<td>49.46</td>
<td>10</td>
<td>101.1</td>
<td>10</td>
</tr>
<tr>
<td>12.4</td>
<td>56.45</td>
<td>20</td>
<td>97.08</td>
<td>15</td>
</tr>
<tr>
<td>12.5</td>
<td>52.48</td>
<td>25</td>
<td>91.01</td>
<td>20</td>
</tr>
<tr>
<td>17.9</td>
<td>61.87</td>
<td>30</td>
<td>77.66</td>
<td>25</td>
</tr>
<tr>
<td>19.1</td>
<td>59.29</td>
<td>eq. 1</td>
<td>S/wt%</td>
<td>30</td>
</tr>
<tr>
<td>22.7</td>
<td>62.37</td>
<td>eq. 1</td>
<td>S/wt%</td>
<td>35</td>
</tr>
<tr>
<td>23.0</td>
<td>57.93</td>
<td>eq. 2</td>
<td>S/wt%</td>
<td>23.0</td>
</tr>
</tbody>
</table>

temp range 274–296 K

\[ \ln \left( \frac{K_H}{\text{atm}} \right) = A - \frac{B}{(T/K)} \]

A = 22.16

B = 4459
**FIGURE 5.1.1.21.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-chlorohexane.

**TABLE 5.1.1.21.2**
Reported vapor pressures of 1-chlorohexane at various temperatures

<table>
<thead>
<tr>
<th>Kemme &amp; Kreps 1969</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Static method-DTA</strong></td>
</tr>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>15.0</td>
</tr>
<tr>
<td>26.7</td>
</tr>
<tr>
<td>33.1</td>
</tr>
<tr>
<td>38.6</td>
</tr>
<tr>
<td>46.7</td>
</tr>
<tr>
<td>52.6</td>
</tr>
<tr>
<td>59.7</td>
</tr>
<tr>
<td>68.4</td>
</tr>
<tr>
<td>79.5</td>
</tr>
<tr>
<td>92.6</td>
</tr>
</tbody>
</table>

*A DTA—differential thermal analyzer
**FIGURE 5.1.1.21.2** Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorohexane.

**FIGURE 5.1.1.21.3** Logarithm of vapor pressure versus reciprocal temperature for 1-chlorohexane.
5.1.1.22 1-Chloroheptane

Common Name: 1-Chloroheptane
Synonym: heptyl chloride
Chemical Name: 1-chloroheptane
CAS Registry No: 629-06-1
Molecular Formula: C_{7}H_{15}Cl
Molecular Weight: 134.647

Melt point (°C):
–69.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point (°C):
160.4 (Lide 2003)

Density (g/cm³):
0.8758, 0.8715 (20°C, 25°C, Dreisbach 1961)
0.8758 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
153.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):
48.19, 37.95 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
13.6 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)
13.6 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
404 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 7.0650 + 1539.35/(208.8 + t/°C); temp range 67–206°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 7.0650 + 1539.35/(208.8 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
680* (34.4°C, differential thermal analysis, measured range 34.4–160°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.83820 − 1410.064/(T/K – 77.511); temp range 307–434 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
4.08 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_\text{1/2}$:

Half-Lives in the Environment:

### TABLE 5.1.1.22.1
Reported vapor pressures of 1-chloroheptane at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>$t/°C$</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>34.4</td>
<td>679.9</td>
<td>127.9</td>
<td>40343</td>
</tr>
<tr>
<td>46.6</td>
<td>1400</td>
<td>145.1</td>
<td>66994</td>
</tr>
<tr>
<td>53.5</td>
<td>2027</td>
<td>160.1</td>
<td>100445</td>
</tr>
<tr>
<td>59.1</td>
<td>2680</td>
<td></td>
<td></td>
</tr>
<tr>
<td>67.5</td>
<td>4013</td>
<td>log P = $A - B/(C + t/°C)$</td>
<td></td>
</tr>
<tr>
<td>73.6</td>
<td>5306</td>
<td>P/mmHg</td>
<td></td>
</tr>
<tr>
<td>81.1</td>
<td>7333</td>
<td>A</td>
<td>6.83820</td>
</tr>
<tr>
<td>90.9</td>
<td>10919</td>
<td>B</td>
<td>1410.064</td>
</tr>
<tr>
<td>101.1</td>
<td>16212</td>
<td>C</td>
<td>195.639</td>
</tr>
<tr>
<td>115.6</td>
<td>27064</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*DTA—differential thermal analyzer

**FIGURE 5.1.1.22.1** Logarithm of vapor pressure versus reciprocal temperature for 1-chloroheptane.
5.1.1.23 1-Chlorooctane

Common Name: 1-Chlorooctane
Synonym: octyl chloride
Chemical Name: 1-chlorooctane
CAS Registry No: 111-85-3
Molecular Formula: C₈H₁₇Cl
Molecular Weight: 148.674
Melting Point (°C):
  -57.8 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
  183.5 (Lide 2003)
Density (g/cm³):
  0.8738, 0.8695 (20°C, 25°C, Dreisbach 1961; Weast 1982–83)
Molar Volume (cm³/mol):
  170.2 (15°C, calculated-density, Stephenson & Malanowski 1987)
  205.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
  53.25, 41.09 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ∆Hᵥ( subprocess) (kJ/mol):
Entropy of Fusion, ∆Sᵥ( subprocess) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  3.67* (generator column-GC, measured range 5–40°C, Sarraute et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  127 (calculated-Antoine eq., Dreisbach 1961)
  log (P:mmHg) = 7.1231 – 1639.2/(204.2 + t°C); temp range 86–231°C (Antoine eq. for liquid state, Dreisbach 1961)
  log (P:mmHg) = 7.1231 – 1369.20/(204.4 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
  747* (54.1°C, differential thermal analysis, measured range 54.1–184.1°C, Kemme & Kreps 1969)
  log (P:mmHg) = 6.84310 – 1469.829/(t°C + 187.157); temp range 54.1–184.1°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)
  118.2 (extrapolated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 5.968 – 1469.829/(T/K – 85.993); temp range 327–457 K (Antoine eq., Stephenson & Malanowski 1987)
  log (P:mmHg) = 7.05152 – 1600.24/(t°C + 200.28); temp range 64–184°C (Antoine eq., Dean 1992)
  126.6* (calculated-Antoine eq. of Li & Rossini 1961, temp range 5–40°C, Sarraute et al. 2004)
Henry’s Law Constant (Pa·m³/mol at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
  4437* (calculated-P/C, temp range 5–40°C, Sarraute et al. 2004)
Octanol/Water Partition Coefficient, log Kₖₐₕ:
  4.48 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)
Octanol/Air Partition Coefficient, log Kₖₐₕ:
Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_1/2$:

Half-Lives in the Environment:

### TABLE 5.1.1.23.1
Reported aqueous solubilities, vapor pressures and Henry’s law constants of 1-chlorooctane at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-GC</td>
<td>Kemme &amp; Kreps 1969</td>
<td>Sarraute et al. 2004</td>
</tr>
<tr>
<td></td>
<td>static method-DTA*</td>
<td>extrapolated -Antoine eq.#</td>
</tr>
<tr>
<td></td>
<td>calculated-P/C</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P$/Pa</th>
<th>$t/°C$</th>
<th>$P$/Pa</th>
<th>$t/°C$</th>
<th>$P$/Pa</th>
<th>$t/°C$</th>
<th>$P$/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.0</td>
<td>3.38</td>
<td>54.1</td>
<td>746.6</td>
<td>5.0</td>
<td>26.30</td>
<td>9.9</td>
<td>26.30</td>
</tr>
<tr>
<td>9.9</td>
<td>3.52</td>
<td>63.9</td>
<td>1307</td>
<td>9.9</td>
<td>39.55</td>
<td>9.9</td>
<td>39.55</td>
</tr>
<tr>
<td>9.9</td>
<td>3.49</td>
<td>72.4</td>
<td>2040</td>
<td>9.9</td>
<td>39.71</td>
<td>9.9</td>
<td>39.71</td>
</tr>
<tr>
<td>9.9</td>
<td>3.36</td>
<td>78.2</td>
<td>2706</td>
<td>9.9</td>
<td>39.71</td>
<td>9.9</td>
<td>39.71</td>
</tr>
<tr>
<td>10.0</td>
<td>3.29</td>
<td>87.1</td>
<td>4040</td>
<td>10.0</td>
<td>40.04</td>
<td>10.0</td>
<td>40.04</td>
</tr>
<tr>
<td>19.1</td>
<td>3.78</td>
<td>93.4</td>
<td>5346</td>
<td>19.1</td>
<td>81.99</td>
<td>19.1</td>
<td>81.99</td>
</tr>
<tr>
<td>25.0</td>
<td>3.67</td>
<td>101.1</td>
<td>7359</td>
<td>25.0</td>
<td>126.6</td>
<td>25.0</td>
<td>126.6</td>
</tr>
<tr>
<td>25.1</td>
<td>3.90</td>
<td>110.7</td>
<td>10732</td>
<td>25.1</td>
<td>127.1</td>
<td>25.1</td>
<td>127.1</td>
</tr>
<tr>
<td>25.2</td>
<td>3.84</td>
<td>121.8</td>
<td>16159</td>
<td>25.2</td>
<td>128.0</td>
<td>25.2</td>
<td>128.0</td>
</tr>
<tr>
<td>30.0</td>
<td>4.03</td>
<td>136.7</td>
<td>27798</td>
<td>30.0</td>
<td>179.8</td>
<td>30.0</td>
<td>179.8</td>
</tr>
<tr>
<td>34.8</td>
<td>4.01</td>
<td>149.8</td>
<td>40210</td>
<td>34.8</td>
<td>248.4</td>
<td>34.8</td>
<td>248.4</td>
</tr>
<tr>
<td>35.1</td>
<td>4.0</td>
<td>167.4</td>
<td>66795</td>
<td>35.1</td>
<td>252.5</td>
<td>35.1</td>
<td>252.5</td>
</tr>
<tr>
<td>35.1</td>
<td>4.16</td>
<td>184.1</td>
<td>103085</td>
<td>35.1</td>
<td>252.5</td>
<td>35.1</td>
<td>252.5</td>
</tr>
<tr>
<td>40.0</td>
<td>4.09</td>
<td>40.0</td>
<td>347.5</td>
<td>40.0</td>
<td>11429</td>
<td>40.0</td>
<td>11429</td>
</tr>
</tbody>
</table>

$\log P = A – B/(T/K)$ (1)  $\ln P = A – B/(T/K)$ (1a)

$\log P = A – B/(C + t/°C)$ (2)  $\ln P = A – B/(C + t/°C)$ (2a)

$\log P = A – B/(C + T/K)$ (3)

$\log P = A – B/(T/K) – C \cdot \log (T/K)$ (4)

**Notes:**
- *DTA—differential thermal analyzer
- Pressure range 10–1500 torr mmHg
**FIGURE 5.1.23.1** Logarithm of vapor pressure versus reciprocal temperature for 1-chlorooctane.
5.1.1.24 1-Chlorononane

Common Name: 1-Chlorononane
Synonym: nonyl chloride
Chemical Name: 1-chlorononane
CAS Registry No: 2473-01-0
Molecular Formula: C₉H₁₉Cl
Molecular Weight: 162.700

Melting Point (°C):

Boiling Point (°C):
205.2 (Lide 2003)

Density (g/cm³):
0.7886 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
206.3 (20°C, calculated-density)
228.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
58.27, 42.89 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, $\Delta H_fus$ (kJ/mol):

Entropy of Fusion, $\Delta S_fus$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

40.0 (extrapolated-Antoine eq., Dreisbach 1961)

$\log (P/\text{mmHg}) = 7.1802 - 1736.11/(200.4 + t/°C)$; temp range 104–255°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/\text{mmHg}) = 7.1802 - 1736.11/(200.4 + t/°C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

680* (69.1°C, differential thermal analysis, measured range 69.1–204.8°C, Kemme & Kreps 1969)

$\log (P/\text{mmHg}) = 6.90463 - 1586.937/(t/°C + 185.505); temp range 69.1–204.8°C$ (Antoine eq. on expntl. data, differential thermal analysis, Kemme & Kreps 1969)

35.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.17172 - 1655.007/(t/°C + 205.166); temp range 69.1–204.8°C$ (Antoine eq., based on expntl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.09107 - 1332.89/(T/K - 54.65); temp range 289–409 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 7.04654 - 1665.57/(t/°C + 192.26); temp range 69–205°C$ (Antoine eq., Dean 1992)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{OW}$:

4.88 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:
### TABLE 5.1.1.24.1
Reported vapor pressures of 1-chlorononane at various temperatures

Kemme & Kreps 1969

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>69.1</td>
<td>679.9</td>
<td>156.7</td>
<td>26731</td>
</tr>
<tr>
<td>70.8</td>
<td>733.3</td>
<td>170.3</td>
<td>40317</td>
</tr>
<tr>
<td>80.6</td>
<td>1280</td>
<td>188.6</td>
<td>66901</td>
</tr>
<tr>
<td>89.9</td>
<td>2013</td>
<td>204.8</td>
<td>100365</td>
</tr>
<tr>
<td>95.4</td>
<td>2613</td>
<td></td>
<td></td>
</tr>
<tr>
<td>104.5</td>
<td>3933</td>
<td></td>
<td></td>
</tr>
<tr>
<td>111.5</td>
<td>5280</td>
<td></td>
<td></td>
</tr>
<tr>
<td>119.8</td>
<td>7333</td>
<td>A</td>
<td>6.94063</td>
</tr>
<tr>
<td>129.5</td>
<td>10626</td>
<td>B</td>
<td>1586.937</td>
</tr>
<tr>
<td>141.3</td>
<td>16159</td>
<td>C</td>
<td>185.505</td>
</tr>
</tbody>
</table>

\[ \log P = A - \frac{B}{(C + t/°C)} \]

*DTA—differential thermal analyzer

### FIGURE 5.1.1.24.1
Logarithm of vapor pressure versus reciprocal temperature for 1-chlorononane.

1-Chlorononane: vapor pressure vs. 1/T

b.p. = 205.2 °C
5.1.1.25  1-Chlorodecane

Common Name: 1-Chlorodecane
Synonym: decyl chloride
Chemical Name: 1-chlorodecane
CAS Registry No: 1002-69-3
Molecular Formula: C\textsubscript{10}H\textsubscript{21}Cl
Molecular Weight: 176.727
Melting Point (°C):
   -31.3 (Dreisbach 1961; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
   225.9 (Lide 2003)
Density (g/cm\textsuperscript{3}):
   0.8705, 0.8666 (20°C, 25°C, Dreisbach 1961)
Molar Volume (cm\textsuperscript{3}/mol):
   203.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
   250.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
   63.35, 45.2 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   13.3 (calculated-Antoine eq., Dreisbach 1961)
   log (P/mmHg) = 7.2372 – 1829.68/(196.6 + t/°C); temp range 121–278°C (Antoine eq. for liquid state, Dreisbach 1961)
   log (P/mmHg) = 7.2372 – 1829.68/(196.6 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
   733* (86.2°C, differential thermal analysis, measured range 86.2–225.6°C, Kemme & Kreps 1969)
   log (P/mmHg) = 6.99172 – 1676.793/(t/°C + 182.017); temp range 86.2–225.6°C (Antoine eq. on exprtl. data, differential thermal analysis, Kemme & Kreps 1969)
   9.85 (extrapolated-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 6.07379 – 1645.521/(t/°C + 178.639); temp range 86.2–225.6°C (Antoine eq. based on exprtl. data of Kemme & Kreps 1969, Boublik et al. 1984)
   log (P\textsubscript{L}/kPa) = 6.11662 – 1676.793/(T/K – 91.133); temp range 359–499 K (Antoine eq., Stephenson & Malanowski 1987)
   log (P/mmHg) = 6.93986 – 1639.06/(t/°C + 177.04); temp range 86–225.9°C (Antoine eq., Dean 1992)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{ow}$:
   5.29 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
TABLE 5.1.1.25.1
Reported vapor pressures of 1-chlorodecane at various temperatures
Kemme & Kreps 1969

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>86.2</td>
<td>733.3</td>
<td>189.5</td>
<td>40183</td>
</tr>
<tr>
<td>98.9</td>
<td>1400</td>
<td>208.6</td>
<td>66861</td>
</tr>
<tr>
<td>106.2</td>
<td>2000</td>
<td>225.6</td>
<td>100618</td>
</tr>
<tr>
<td>112.8</td>
<td>2693</td>
<td></td>
<td></td>
</tr>
<tr>
<td>122.7</td>
<td>4106</td>
<td>log P = A – B/(C + t/°C)</td>
<td></td>
</tr>
<tr>
<td>129.2</td>
<td>5346</td>
<td></td>
<td></td>
</tr>
<tr>
<td>137.1</td>
<td>7293</td>
<td>P/mmHg</td>
<td></td>
</tr>
<tr>
<td>147.7</td>
<td>10666</td>
<td>A</td>
<td></td>
</tr>
<tr>
<td>159.3</td>
<td>16065</td>
<td>B</td>
<td></td>
</tr>
<tr>
<td>175.7</td>
<td>26878</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*DTA—differential thermal analyzer

FIGURE 5.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorodecane.
5.1.1.26 Chloroethene (Vinyl chloride)

Common Name: Vinyl Chloride
Synonym: chloroethene, chloroethylene, monochloroethylene, monovinylchloride, MVC
Chemical Name: chloroethylene, vinyl chloride, chloroethene
CAS Registry No: 75-01-4
Molecular Formula: C₂H₃Cl, H₂C = CHCl
Molecular Weight: 62.498
Melting Point (°C):
-153.84 (Lide 2003)
Boiling Point (°C):
-13.8 (Lide 2003)
Density (g/cm³ at 20°C):
0.9106 (Riddick et al. 1986)
Molar Volume (cm³/mol):
68.5 (20°C, Stephenson & Malanowski 1987)
65.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔH₟ (kJ/mol):
4.745 (Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS₟ (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
8720, 9000 (15, 30°C, shake flask-interferometry, Gross & Saylor 1931)
2700* (continuous solvent flow system at 1 atmospheric pressure, measured range 0.2–75°C, Hayduk & Laudie 1974)
60 (10°C, Pearson & Connell 1975)
60, 2700 (10, 25°C, selected, Dilling 1977)
1100 (Verschueren 1977, 1983)
6800 (20°C, selected, Nathan 1978)
8700* (restatement of Hayduk & Laudie 1974, temp range 0.2–75°C at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)
8800* (26°C, solubility bomb-headspace GC, measured range 15–85°C at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)
2763* (recommended, temp range 0–175°C, Horvath 1982)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
538000* (Antoine eq. regression, temp range −105.6 to −13.8°C, Stull 1947)
354600 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.49712 − 783.4/(230.0 + t°C), temp range −100 to 50°C (Antoine eq. for liquid state, Dreisbach 1959)
104698* (−13.00°C, ebulliometry, measured range −64.9 to −13.00°C, McDonald et al. 1959)
381600 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 6.88054 − 912.5/(242.0 + t°C); temp range −73 to 46°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.86108 − 892.757/(238.099 + t°C); temp range −64.9 to 13.0°C (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)
172719* (0°C, temp range −59.4 to 0°C, Huccura & Mathieu 1967)

546800 (calculated-Antoine eq., Weast 1972–73)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 6263.0/(T/\text{K})] + 8.202782; \text{ temp range} -105.1 \text{ to } -13.8^\circ\text{C} (\text{Antoine eq., Weast 1972–73})
\]

392800 (calculated-Antoine eq., Boublík et al. 1973)
\[
\log (P/\text{mmHg}) = 6.89117 – 905.008/(239.475 + t/^\circ\text{C}); \text{ temp range} –64.9 \text{ to } –13.0^\circ\text{C} (\text{Antoine eq. from reported expl. data, Boublík et al. 1973})
\]

309300 (Pearson & McConnell 1975)
\[
\log (P/\text{mmHg}) = 6.89117 – 905.01/(239.48 + t/^\circ\text{C}); \text{ temp range not specified} (\text{Antoine eq., Dean 1985, 1992})
\]

387000 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = 6.89117 – 905.01/(239.475 + t/^\circ\text{C}); \text{ temp range} 208–260 \text{ K} (\text{Antoine eq.-I, Stephenson & Malanowski 1987})
\]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5680 (exptl.-1/K Aw = Cw/CA, Hine & Mookerjee 1975)

4723 (calculated-bond contribution method, Hine & Mookerjee 1975)

117705 (10°C, Pearson & McConnell 1975)

39660 (calculated-P/C, Neely 1976)

106590 (calculated-P/C, Dilling 1977)

2350 (calculated-P/C, Mackay & Shiu 1981)

2817* (24.8°C, EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)
\[
\ln [H/(\text{atm m}^3/\text{mol})] = 7.385 – 3286/(T/\text{K}); \text{ temp range} 10.3–34.6^\circ\text{C} (\text{EPICS measurements, Gossett 1987})
\]

2685* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
\[
\ln [H/(\text{atm m}^3/\text{mol})] = 6.138 – 2931/(T/\text{K}); \text{ temp range} 10–30^\circ\text{C} (\text{EPICS measurements, Ashworth et al. 1988})
\]

2271 (computed value, Yaws et al. 1991)

2172 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
\[
\log K_{Aw} = 4.119 – 1223/(T/\text{K}) \text{ (summary of literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, log K_{ow}:
\[
1.39 \text{ (calculated-π substituent const., Hansch et al. 1968)}
\]
\[
0.60 \text{ (Callahan et al. 1979; Mills et al. 1982)}
\]
\[
1.23 \text{ (calculated-fragment const., Mabey et al. 1982)}
\]
\[
2.79 \text{ (Hansch et al. 1995)}
\]

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:
\[
0.845 \text{ (estimated-S, Lyman et al. 1982)}
\]
\[
0.756 \text{ (microorganisms-water, calculated-K_{ow}, Mabey et al. 1982)}
\]
\[
3.04, 1.60, < 1.0 \text{ (activated sludge, Chlorella fusca, golden ide, Freitag et al. 1984)}
\]
\[
0.068 \text{ (from USEPA 86, Yeh & Kastenberg 1991)}
\]

Sorption Partition Coefficient, log K_{oc}:
\[
0.9138 \text{ (sediment-water, calculated-K_{ow}, Mabey et al. 1982)}
\]
\[
1.748 \text{ (estimated-S, Lyman et al. 1982)}
\]
\[
0.477 \text{ (soil, selected, Jury et al. 1990)}
\]
\[
1.756 \text{ (quoted from USEPA 1986, Yeh & Kastenberg 1991)}
\]
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volutilization: $t_{1/2} = 25$ min from water, by rapidly stirring aqueous solutions in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

$t_{1/2}(\text{exptl}) = 27.6$ min, $t_{1/2}(\text{calc}) = 0.0054$ min, 16.1 min from water at 10°C (Dilling 1977)

$t_{1/2} \approx 0.805$ h for volatilization from a river of 1-m deep with a current of 3 m/s and wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

estimated $t_{1/2} = 0.2$ to 0.5 d from soil at 1 and 10 cm incorporation (Jury et al. 1984);

Volatilization $t_{1/2} = 30$ d, estimated volatilization from soil (Jury et al. 1990).

Photolysis: degrade rapidly in air by reaction with photochemically produced hydroxyl radicals with an estimated $t_{1/2} = 1.5$ d (Perry et al. 1977; quoted, Howard 1989).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 26°C (Perry et al. 1977)

$k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979,1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{O3} = 6.5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Sanhueza et al. 1976; quoted, Atkinson & Carter 1984)

$k_{O3} = 2.3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Gay et al. 1976; quoted, Atkinson & Carter 1984)

$k_{O3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979,1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 1.8 d, loss of 42.6% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}(\text{calc}) = 3.9 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{O3} = 1.2 \times 10^{6} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and 3.0 M$^{-1}$ h$^{-1}$ for peroxo radical at 25°C (Mabey et al. 1982)

$k_{OH} = (2.45 \pm 0.45) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zhang et al. 1983; quoted, Atkinson & Carter 1984)

$k_{OH} = (3.30 \pm 1.66) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 1 K (Anderson & Ljungström 1989)

$k_{OH} = (2.30 \pm 1.1) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{NO3} = 2.30 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculate atmospheric lifetime $\tau = 42$ d, and $k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 3.5$ d and $k_{O3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 66$ d at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1991)

$k_{NO3} = (3.30 \pm 1.66) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 1 K (quoted from Anderson & Ljungström 1989, Atkinson 1991)

$k_{NO3} = 4.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljic & Güsten 1990)

$k_{NO3} = 4.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH}(\text{calc}) = 5.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis: $t_{1/2} < 10$ yr (Callahan et al. 1979);

estimated acid-catalyzed rate constant of $3.30 \times 10^{-12} \text{ mol}^{-1} \text{ s}^{-1}$ at pH 5 with calculated $t_{1/2} = 2 \times 10^{11}$ d (Wolfe 1980; quoted, Ma et al. 1990)

abiotic hydrolysis or dehydrohalogenation $t_{1/2} < 120$ months (Olsen & Davis 1990).

Biodegradation: abiotic degradation rate constant of $k = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 26°C determined in laboratory experiments for the vapor phase reaction with hydroxyl radicals (Perry et al. 1977; quoted, Howard 1989)

$t_{1/2}(\text{aq. aerobic}) = 672$–4320 h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991)
greater than 99% degraded after 108 d under aerobic conditions and approximately 65% being mineralized to $^{14}$CO$_2$ under aerobic conditions (Davis & Carpenter 1990);

$t_{1/2}$ (aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60$ d (Olsen & Davis 1990)

$t_{1/2}$ (aerobic) = 28 d, $t_{1/2}$ (anaerobic) = 110 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 11$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 0.24$–2.4 h from air for the reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 4.3$ h with NO under simulated atmospheric conditions (Dilling et al. 1976);

estimated $t_{1/2} = 1.5$ d, based on its photochemical reaction with OH radical in air (Perry et al. 1977; quoted, Howard 1989);

residence time of 1.8 d, loss of 42.6% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

$t_{1/2} = 9.7$–97 h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes $\tau = 42$ d for the reaction with NO$_3$ radical for a 12-h nighttime, average concn. of $2.4 \times 10^9$ molecule/cm$^3$; $\tau = 3.5$ d for the reaction with OH radical for a 12-h average concn. of $1.0 \times 10^6$ molecule/cm$^3$, and $\tau = 66$ d for the reaction with O$_3$ for a 24-h, average concn. of $7 \times 10^{11}$ molecule/cm$^3$ (Atkinson et al. 1987).

Surface water: estimated $t_{1/2} = 0.805$ h for volatilization from a river of 1 m deep with a current of 3 m/s and a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 672$–4320 h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 1344$–69000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and an estimated half-life for anaerobic biodegradation from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2} = 0.2$ to 0.5 d for volatilization from soil at 1 and 10 cm incorporation (Jury et al. 1984; quoted, Howard 1989);

$t_{1/2} = 30$ d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 30$–180 d (Howard et al. 1991; quoted, Jury et al. 1992);

$t_{1/2} = 672$–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988; quoted, Jury et al. 1992).
### TABLE 5.1.1.26.1
Reported aqueous solubilities of chloroethene (vinyl chloride) at various temperatures

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>compressibility apparatus</td>
<td>“restatement” data</td>
<td>solubility bomb-GC/FID</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>at 1.0 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>7537</td>
<td>0.2</td>
<td>9000</td>
<td>0</td>
</tr>
<tr>
<td>25</td>
<td>2700</td>
<td>25</td>
<td>8700</td>
<td>16</td>
</tr>
<tr>
<td>50</td>
<td>1278</td>
<td>50</td>
<td>10100</td>
<td>20.5</td>
</tr>
<tr>
<td>75</td>
<td>507</td>
<td>75</td>
<td>12800</td>
<td>26</td>
</tr>
<tr>
<td>at 1.36 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>8438</td>
<td># “restatement” data</td>
<td>35</td>
<td>9400</td>
</tr>
<tr>
<td>at 3.06 atm</td>
<td></td>
<td>from Hayduk &amp; Laudie 1974</td>
<td></td>
<td>41</td>
</tr>
<tr>
<td>25</td>
<td>7153</td>
<td></td>
<td>46.5</td>
<td>8800</td>
</tr>
<tr>
<td>50</td>
<td>3993</td>
<td></td>
<td>55</td>
<td>9500</td>
</tr>
<tr>
<td>75</td>
<td>2125</td>
<td></td>
<td>65</td>
<td>9200</td>
</tr>
<tr>
<td>at 6.12 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>7674</td>
<td></td>
<td>72.5</td>
<td>9800</td>
</tr>
<tr>
<td>75</td>
<td>4965</td>
<td></td>
<td>80</td>
<td>10000</td>
</tr>
<tr>
<td>$\Delta H_{sol}$(kJ mol$^{-1}$) at 25°C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.26.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for chloroethene.
### TABLE 5.1.1.26.2
Reported vapor pressures of chloroethene (vinyl chloride) at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C\log(T/K) \quad (4) \\
\log P &= A - \frac{B}{T/K} - C(T/K) + D(T/K)^2 \quad (5)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Source</th>
<th>Data Type</th>
<th>Table Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stull 1947</td>
<td>summary</td>
<td>t/°C  P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-103.6    133.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-90.8     666.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-83.7     1333</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-75.7     2666</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-66.8     5333</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-61.1     7999</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-53.2     13332</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-41.3     26664</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-28.0     53329</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-13.8     101325</td>
</tr>
<tr>
<td></td>
<td>ebulliometry</td>
<td>t/°C  P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-59.4     9870</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-54.3     13566</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-49.4     18032</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-44.5     23713</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-39.5     31881</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-34.5     39695</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-29.65    50510</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-24.9     63349</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-20.1     78440</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0       172719</td>
</tr>
</tbody>
</table>

**mp/°C** -153.7

**FIGURE 5.1.1.26.2** Logarithm of vapor pressure versus reciprocal temperature for chloroethene.
TABLE 5.1.1.26.3
Reported Henry's law constants of chloroethene (vinyl chloride) at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)
\]

\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)
\]

\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)
\]

\[
\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \quad \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)
\]

\[
K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)
\]

Hayduk & Laudie 1974

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>834</td>
<td>10.3</td>
<td>1489</td>
</tr>
<tr>
<td>25</td>
<td>2342</td>
<td>17.5</td>
<td>1956</td>
</tr>
<tr>
<td>50</td>
<td>4348</td>
<td>24.8</td>
<td>2819</td>
</tr>
<tr>
<td>75</td>
<td>7751</td>
<td>34.6</td>
<td>3627</td>
</tr>
</tbody>
</table>

at 1 atm

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>0.2</th>
<th>1018</th>
<th>eq. 4a</th>
<th>H/(atm m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2685</td>
<td>7.385</td>
<td>A</td>
<td>7.385</td>
<td>A</td>
</tr>
<tr>
<td>50</td>
<td>4669</td>
<td>3286</td>
<td>B</td>
<td>6.138</td>
<td>B</td>
</tr>
<tr>
<td>75</td>
<td>7988</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

at 1.36 atm

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>30</th>
<th>3850</th>
</tr>
</thead>
</table>

FIGURE 5.1.1.26.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethene.
5.1.1.27 1,1-Dichloroethene

\[
\begin{align*}
\text{Cl} & \quad \text{Cl} \\
\end{align*}
\]

Common Name: 1,1-Dichloroethene
Synonym: 1,1-dichloroethene, vinylidene chloride, vinylidine chloride, 1,1-DCE
Chemical Name: 1,1-dichloroethene, 1,1-dichloroethylene
CAS Registry No: 75-35-4
Molecular Formula: \( \text{C}_2\text{H}_2\text{Cl}_2, \text{CH}_2 = \text{CCl}_2 \)
Molecular Weight: 96.943
Melting Point (°C): 
-122.56 (Lide 2003)
Boiling Point (°C): 
31.6 (Lide 2003)
Density (g/cm³ at 20°C):
1.2180 (Horvath 1982; Weast 1982–83; Verschueren 1983)
1.2132 (Riddick et al. 1986)
Molar Volume (cm³/mol):
79.9 (20°C, calculated-density)
86.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
26.49, 28.18 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
6.514 (Riddick et al. 1986)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, \( F \): 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
400 (20°C, shake flask-GC, McConnell et al. 1975; Pearson & McConnell 1975)
400 (20°C, literature average, Dilling 1977)
2250* (solubility bomb-headspace GC, measured range 15–90.5°C, DeLassus & Schmidt 1981)
210* (summary of literature data, Horvath 1982)
2640, 3675 (20°C, 30°C, saturation concn., Verschueren 1983)
2232 (30°C, headspace-GC, McNally & Grob 1984)
210 (Dean 1985; Riddick et al. 1986)
2843, 2790, 2782 (20, 30, 40°C, infinite dilution activity coeff. \( \gamma^{-}\)-GC, Tse et al. 1992)
2420* (recommended, temp range 0–90°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
\[
S/(\text{wt}%) = 6.27413 - 3.8257 \times 10^{-2}(T/K) + 6.04607 \times 10^{-5}(T/K)^2, \text{ temp range 288–363 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)}
\]

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
86430* (Antoine eq. regression, temp range –77.2 to 31.7°C, Stull 1947)
97241* (30.39°C, ebulliometry, measured range –28.36 to 32.50°C, Hildebrand et al. 1959)
84500 (calculated-Antoine eq., Weast 1972–73)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 7211.8/(T/K)] + 8.087140; \text{ temp range } -77.2 \text{ to } 31.7^\circ \text{C (Antoine eq., Weast 1972–73)}
\]
80040 (calculated-Antoine eq., Boublik et al. 1973)
\[
\log (P/\text{mmHg}) = 6.97215 - 1099.446/(237.184 + t^\circ \text{C}); \text{ temp range } -28 \text{ to } 32.5^\circ \text{C (Antoine eq. from reported exptl. data, Boublik et al. 1973)}
\]
79710 (literature average, Dilling 1977)
78780 (Verschueren 1977,1983)
Halogenated Aliphatic Hydrocarbons

80040 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.09904 – 1100.431/(237.274 + t°C); temp range –28 to 32.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9722 – 1099.4/(237.2 + t°C); temp range –28 to 32°C (Antoine eq., Dean 1985, 1992)
79860 (selected, Riddick et al. 1986)
log (P/kPa) = 6.10690 – 1104.29/(237.697 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
80060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.10046 – 1100.67/(–35.9 + T/K); temp range 244–306 K (Antoine eq., Stephenson & Malanowski 1987)
66190, 95740, 134520 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = –16.5419 – 1.6655 × 10³/(T/K) + 13.923·log (T/K) – 4.0958 × 10⁻²·(T/K) + 2.9995 × 10⁻⁵·(T/K)²; temp range 151–482 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3729 (20°C, batch stripping, Mackay et al. 1979)
3127* (24.3°C, equilibrium cell-concn ratio, measured range 2.5–26.1°C, Leighton & Calo 1981)
ln (kH/atm) = 23.12 – 4618/(T/K); temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
2649 (20°C, EPICS-GC, Linoff & Gossett 1983; Gossett 1985)
2645 (24.8°C, EPICS-GC, measured range 10–34.6°C, Gossett 1987)
1520 (gas stripping-GC, Warner et al. 1987)
7529 (20°C, EPICS-GC, Yurteri et al. 1987)
2624* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m³/mol)] = 8.845 – 3729/(T/K); temp range 10.0–34.6°C (EPICS measurements, Gossett 1987)
2136 (computed value, Yaws et al. 1991)
2320, 3415, 4813 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
2376 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log Kₐw = 5.397 – 1586/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kₐw:
2.13 (shake flask, Log P Database, Hansch & Leo 1987)
2.13 (recommended, Sangster 1993)
2.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₒa:

Bioconcentration Factor, log BCF:
1.72 (microorganisms-water, calculated-Kₐw, Mabey et al. 1982)

Sorption Partition Coefficient, log Kₒc:
2.176 (calculated-Kₐw, Kenaga & Goring 1980)
1.813 (sediment-water, calculated-Kₒc, Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, tₜ/₂:
Volatilization: tₒv(calc) ~ 22 min at 25°C for volatilization of 1 mg/L in water in an open container of 65-mm depth stirring at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)
Evaporation tₒe(calc) = 27.2 min, tₒe(calc) = 0.029 min, 20.1 min from water (Dilling 1977)
Evaporation tₒe(calc) = 5.9, 1.2, and 4.7 d from a pond, river, and lake, respectively, using data for the oxygen reaeration rate of typical bodies of water (Mill et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kₒh for reaction with OH radical, kₒₙₒ₃ with NO₃ radical and kₒₒ₃ with O₃ or as indicated, *data at other temperatures see reference:
$k_{O_3} = (3.7 \pm 1.0) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Hull et al. 1973; quoted, Atkinson & Carter 1984)

Photooxidation $t_{1/2} \approx 50 \text{ min}$ reaction with NO$_2$ under UV irradiation (Gay, Jr. et al. 1976)

$k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $3.0 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k_{OH} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 2.9 d, loss of 29.2% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k \approx 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1.5 mM $t$-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (3.7 \pm 1.0) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH} = (14.9 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to n-butane at 22.3 ± 1.2°C with a lifetime of 0.75 d and $k_{OH} = 15.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to n-pentane at 24.4 ± 0.4°C (relative rate method, Edney et al. 1986)

$k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH} = (14.9 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to n-butane at 22.3 ± 1.2°C with a lifetime of 0.75 d and $k_{OH} = 15.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to n-pentane at 24.4 ± 0.4°C (relative rate method, Edney et al. 1986)

$k_{NO_3} = (6.60 \pm 3.10) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{NO_3} = 6.6 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 15 d, $k_{OH} = 8.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 3.4 d and $k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 12 yr at room temp. (Atkinson et al. 1987; quoted, Sabljic & Güsten 1990)

$k_{OH} = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 8.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{O_3} = 1.28 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{O_3} = 1.23 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (Atkinson 1991)

$k_{OH} = 2.04 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{OH} = 2.67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis: estimated acid-catalyzed rate constant $k = 1.4 \times 10^{-13} \text{ mol}^{-1} \text{ s}^{-1}$ at pH 5 with $t_{1/2} = 6 \times 10^2 \text{ d}$ at pH 5 (Wolfe 1980);

estimated $t_{1/2} \approx 2.0 \text{ yr}$ at pH 7.0 (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

$\tau_{OH} = 6–9$ months has been observed with no significant difference in hydrolysis rate between pH 4.5 and 8.5 (Cline & Delfino 1987; quoted, Howard 1989);

abiotic hydrolysis or dehydrohalogenation half-life of 12 months (Olsen & Davis 1990).

Biodegradation: aerobic $t_{1/2} = 672–4320 \text{ h}$, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{1/2} = 1944–4152 \text{ h}$, based on anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard 1989; Olsen & Davis 1990; Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 8.0 \text{ wk}$, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 0.24–2.4 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition $t_{1/2} = 2.1 \text{ h}$ with NO under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation $t_{1/2} = 11 \text{ h}$ in relatively clean air (Edney et al. 1983; quoted, Howard 1989) or under 2 h in polluted air (Howard 1989);

lifetime of 0.75 d, based on measured rate data for the vapor phase reaction with OH radical in air at (22.3 ± 1.2°C (Edney et al. 1986);

$t_{1/2} = 9.9–98.7 \text{ h}$, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991);

atmospheric lifetimes: 15 d for the reaction with NO$_3$ radical for a 12-h nighttime average concn. of $2.4 \times 10^9 \text{ molecule cm}^{-3}$, 3.4 d for the reaction with OH radical for a 12-h average concentration...
of \(1.0 \times 10^6\) molecule cm\(^{-3}\), and 12 yr for the reaction with \(O_3\) for a 24-h average concentration of \(7 \times 10^{11}\) molecule cm\(^{-3}\) at room temp. (Atkinson et al. 1987).

Surface water: \(t_{1/2} = 672-4320\) h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: \(t_{1/2} = 1344-3168\) h, based on estimated aqueous aerobic biodegradation half-life and anaerobic grab sample data for soil from ground water aquifer receiving landfill leachate (Wilson et al. 1986; quoted, Howard et al. 1991).

Sediment:

Soil: \(t_{1/2} = 672-4320\) h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

\(t_{1/2} < 10\) d (Ryan et al. 1988).

Biota: \(t_{1/2} < 10\) d, subject to plant uptake via volatilization (Ryan et al. 1988).

<table>
<thead>
<tr>
<th>TABLE 5.1.27.1</th>
<th>Reported aqueous solubilities of 1,1-dichloroethene at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>solubility bomb-GC/FID</strong></td>
<td><strong>summary of literature data</strong></td>
</tr>
<tr>
<td>(t/°C)</td>
<td>S/g·m(^{-3})</td>
</tr>
<tr>
<td>15</td>
<td>2400</td>
</tr>
<tr>
<td>17</td>
<td>2550</td>
</tr>
<tr>
<td>20.5</td>
<td>2500</td>
</tr>
<tr>
<td>25</td>
<td>2250</td>
</tr>
<tr>
<td>28.5</td>
<td>2400</td>
</tr>
<tr>
<td>29.5</td>
<td>2550</td>
</tr>
<tr>
<td>38.5</td>
<td>2200</td>
</tr>
<tr>
<td>45</td>
<td>2100</td>
</tr>
<tr>
<td>51</td>
<td>2300</td>
</tr>
<tr>
<td>55</td>
<td>2100</td>
</tr>
<tr>
<td>60</td>
<td>2400</td>
</tr>
<tr>
<td>65</td>
<td>2250</td>
</tr>
<tr>
<td>71</td>
<td>2950</td>
</tr>
<tr>
<td>74.5</td>
<td>2500</td>
</tr>
<tr>
<td>81</td>
<td>2950</td>
</tr>
<tr>
<td>85.5</td>
<td>3700</td>
</tr>
<tr>
<td>90.5</td>
<td>3500</td>
</tr>
<tr>
<td>eq. 1</td>
<td>S/wt%</td>
</tr>
<tr>
<td>temp range 288–363 K</td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 5.1.1.27.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.2
Reported vapor pressures of 1,1-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

\[ \log P = A - \frac{B}{T/K} \] (1)

\[ \ln P = A - \frac{B}{T/K} \] (1a)

\[ \log P = A - \frac{B}{C + t/°C} \] (2)

\[ \ln P = A - \frac{B}{C + t/°C} \] (2a)

\[ \log P = A - \frac{B}{C + t/°C} - C \cdot \log (T/K) \] (3)

\[ \log P = A - \frac{B}{T/K} - C \cdot (T/K) + D \cdot (T/K)^2 \] (4)

\[ \log P = A - \frac{B}{T/K} - C \cdot (T/K) + D \cdot (T/K)^2 \] (5)

<table>
<thead>
<tr>
<th>Summary of literature data</th>
<th>Hildenbrand et al. 1959</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>-77.2</td>
<td>133.3</td>
</tr>
<tr>
<td>-60.0</td>
<td>666.6</td>
</tr>
<tr>
<td>-51.2</td>
<td>1333</td>
</tr>
<tr>
<td>-41.7</td>
<td>2666</td>
</tr>
<tr>
<td>-31.1</td>
<td>5333</td>
</tr>
<tr>
<td>-24.0</td>
<td>7999</td>
</tr>
<tr>
<td>-15.0</td>
<td>13332</td>
</tr>
<tr>
<td>-1.0</td>
<td>26664</td>
</tr>
<tr>
<td>14.8</td>
<td>53329</td>
</tr>
<tr>
<td>31.7</td>
<td>101325</td>
</tr>
</tbody>
</table>

mp/°C -122.5
### FIGURE 5.1.1.27.2
Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethene.

### TABLE 5.1.1.27.3
Reported Henry's law constants of 1,1-dichloroethene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry's Law Constant</th>
<th>Equation</th>
<th>Constants</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ln K_{AW} = A - \frac{B}{T/K} )</td>
<td>(1)</td>
<td>( A ), ( B )</td>
<td>( K_{AW} )</td>
</tr>
<tr>
<td>( \log K_{AW} = A - \frac{B}{T/K} )</td>
<td>(1a)</td>
<td>( A ), ( B )</td>
<td>( K_{AW} )</td>
</tr>
<tr>
<td>( \ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} )</td>
<td>(2)</td>
<td>( A ), ( B )</td>
<td>( 1/K_{AW} )</td>
</tr>
<tr>
<td>( \log \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} )</td>
<td>(2a)</td>
<td>( A ), ( B )</td>
<td>( 1/K_{AW} )</td>
</tr>
<tr>
<td>( \ln \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] = A - \frac{B}{T/K} )</td>
<td>(3)</td>
<td>( A ), ( B )</td>
<td>( H_{\text{atm}} )</td>
</tr>
<tr>
<td>( \log \left[ \frac{H}{(\text{atm m}^3/\text{mol})} \right] = A - \frac{B}{T/K} )</td>
<td>(3a)</td>
<td>( A ), ( B )</td>
<td>( H_{\text{atm}} )</td>
</tr>
<tr>
<td>( K_{AW} = A - B \frac{(T/K)}{} + C \frac{(T/K)^2}{\cdot} )</td>
<td>(4)</td>
<td>( A ), ( B ), ( C )</td>
<td>( K_{AW} )</td>
</tr>
</tbody>
</table>

#### Equilibrium Cell-GC
<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/(\text{Pa m}^3/\text{mol}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>973</td>
</tr>
<tr>
<td>7.0</td>
<td>1423</td>
</tr>
<tr>
<td>12.9</td>
<td>2119</td>
</tr>
<tr>
<td>18.0</td>
<td>2437</td>
</tr>
<tr>
<td>19.5</td>
<td>3195</td>
</tr>
<tr>
<td>24.3</td>
<td>3127</td>
</tr>
<tr>
<td>26.1</td>
<td>3914</td>
</tr>
</tbody>
</table>

#### EPICS-GC
<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/(\text{Pa m}^3/\text{mol}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>1287</td>
</tr>
<tr>
<td>17.5</td>
<td>1935</td>
</tr>
<tr>
<td>24.8</td>
<td>2645</td>
</tr>
<tr>
<td>34.6</td>
<td>3708</td>
</tr>
<tr>
<td></td>
<td>eq. 4a</td>
</tr>
<tr>
<td>A</td>
<td>8.845</td>
</tr>
<tr>
<td>B</td>
<td>3729</td>
</tr>
</tbody>
</table>

#### EPICS-GC
<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/(\text{Pa m}^3/\text{mol}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1560</td>
</tr>
<tr>
<td>15</td>
<td>2057</td>
</tr>
<tr>
<td>20</td>
<td>2209</td>
</tr>
<tr>
<td>25</td>
<td>2624</td>
</tr>
<tr>
<td>30</td>
<td>3222</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/(\text{atm m}^3/\text{mol}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>eq. 3</td>
<td>( H/\text{atm} )</td>
</tr>
<tr>
<td>A</td>
<td>23.12</td>
</tr>
<tr>
<td>B</td>
<td>4618</td>
</tr>
</tbody>
</table>

Leighton & Calo 1981
Gossett 1987
Ashworth et al. 1988
Tse et al. 1992

© 2006 by Taylor & Francis Group, LLC
FIGURE 5.1.27.3 Logarithm of Henry’s law constant versus reciprocal temperature for 1,1-dichloroethene.
5.1.1.28 cis-1,2-Dichloroethene

Common Name: cis-1,2-Dichloroethylene
Synonym: cis-acetylene dichloride, cis-1,2-dichloroethene, cis-1,2-dichloroethylene, (Z)-1,2-dichloroethene
Chemical Name: cis-1,2-dichloroethene, cis-1,2-dichloroethylene
CAS Registry No: 156-59-2
Molecular Formula: C₂H₂Cl₂, CHCl=CHCl
Molecular Weight: 96.943
Melting Point (°C):
-80.0 (Lide 2003)
Boiling Point (°C):
60.1 (Lide 2003)
Density (g/cm³ at 20°C):
1.2837 (Horvath 1982; Weast 1982–83; Riddick et al. 1986)
1.2818 (Dean 1985)
Molar Volume (cm³/mol):
75.52 (20°C, calculated-density)
86.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
31.57, 30.23 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔHfus (kJ/mol):
7.205 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3520 (Seidell 1940)
3500 (selected from literature or measured in DuPont laboratories, McGovern 1943)
5560 (37°C, shake flask-GC, Sato & Nakijima 1979)
3500 (summary of literature data, Horvath 1982)
7700 (Dean 1985)
6575, 6707, 6674 (20, 30, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)
6292, 6092, 6220 (20, 30, 40°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
6608 (20°C, limiting activity coeff. γ∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
6410* (tentative values, measured range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 27.7353 – 0.178316·(T/K) + 2.93282 × 10⁻⁴·(T/K)², temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25571* (23.74°C, temp range 0.76–83.63°C, Ketelaar et al. 1947)
27260* (interpolated-Antoine eq. regression, temp range −58.4 to 59°C, Stull 1947)
28984* (dynamic-ebulliometry, measured range 19.2–62°C, Flom et al. 1951)
23540 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7420.6/(T/K)] + 7.685137; temp range −58.4 to 260°C (Antoine eq., Weast 1972–73)
27010 (calculated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.0233 – 1105.436/(230.62 + t°C); temp range 0.76–83°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
27010, 26740 (interpolated-Antoine equations; Boublik et al. 1984)
log (P/kPa) = 6.14603 – 1204.804/(230.55 + t°C); temp range 0.76–83.63°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.03144 – 1153.738/(222.905 + t°C); temp range 19.2–62°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.0223 – 1205.4/(230.6 + t°C); temp range 0–84°C (Antoine eq., Dean 1985, 1992)

26700 (selected, Riddick et al. 1986)

log (P/kPa) = 6.9771 – 1651.52/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)

26980 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.30025 – 1293.95/(–32.41 + T/K); temp range 273–334 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.22178 – 1271.55/(–30.557 + T/K); temp range 332–495 K (Antoine eq.-II, Stephenson & Malanowski 1987)

21710, 33305, 49350 (20, 30, 40°C, estimated, Tse et al. 1992)

log (P/mmHg) = 55.9403 – 3.1677 × 103/(T/K) –18.572·log (T/K) + 9.8828 × 10–3·(T/K) + 5.7644 × 10–14·(T/K)²; temp range 193–527 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

342.2 (exptl.-1/K AW = C_W/C_A, Hine & Mookerjee 1975)
1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
444 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
413.4* (EPICS-GC, measured range 10.3–34.6°C, Gossett 1987)

ln [H/(atm m³/mol)] = 8.479 – 4192/(T/K); temp range 10.3–34.6°C (EPICS measurements, Gossett 1987)
441.1 (20°C, EPICS, Yurteri et al. 1987)
460* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m³/mol)] = 5.164 – 3143/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
745.5 (computed value, Yaws et al. 1991)
324, 496, 740 (20, 30, 40°C, infinite dilution activity coeff. γ–GC, Tse et al. 1992)
331, 518, 751 (20, 30, 40°C, activity coeff. γ–differential pressure transducer, Wright et al. 1992)
319 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
674.5 (modified EPICS method-GC, Ryu & Park 1999)
341 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)


Octanol/Water Partition Coefficient, log K OW:
1.86 (shake flask, Hansch & Leo 1985, 1987)
1.86 (recommended, Sangster 1993)
1.85 (infinite dilution activity coefficient-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, log K OA:
2.56 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.176 (calculated-K OW, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K OC:
1.69 (calculated-K OW, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k and Half-Lives, t ½:
V olatilization: evaporation t ½ = 18 min from dilute aqueous solution (Dilling 1975);
Evaporation t ½(exptl) = 19.4 min, t ½(calc) = 0.75 min, 20.7 min from water (Dilling 1977);

V_t = 19.4 min from a slowly stirred beaker 6.5 cm deep equivalent to t ½ = 5.0 h in a body of water 1 m deep (Dilling 1977; quoted, Verschueren 1983; Howard 1990)

V t = 3.1 h was estimated from Henry’s law constant for a model river 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{O3} = 6.2 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{OH} = 4.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{O3} < 5.0 \times 10^{-21}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{O3} = 3.7 \times 10^{10}$ cm$^-1$ mol$^{-1}$ s$^{-1}$, was estimated at 300 K (Lyman 1982)

$k < 800$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{O3} = 6.2 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH} = 4.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{O3} = 5.0 \times 10^{-21}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{O3} = 6.2 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH} = 4.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson et al. 1991)

$k_{O3} = (7.5 \pm 3.5) \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson et al. 1991)

$k_{O3} = 7.5 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated atmospheric lifetime of 130 d, $k_{OH} = 2.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a lifetime of 12 d, and $k_{O3} < 5 \times 10^{-21}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a lifetime of > 9 yr at room temp. (Atkinson et al. 1987)

$k_{OH} = 2.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, was estimated at 298 ± 2 K (relative rate method, Atkinson 1987; quoted, Howard et al. 1991; Sabljic & Güsten 1990)

$k_{OH} = 1.46 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{OH} = (2.38 \pm 0.14) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (relative rate method, Tuazon et al. 1988)

$k_{O3} = (1.39 \pm 0.13) \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (Atkinson 1991)

$k_{OH} = 2.24 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{O3(aq.)} = (310 \pm 20)$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2, with $t_{1/2} = 1.8$ min at pH 7 and 25°C (Yao & Haag 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672–4320$ h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{1/2} = 2688–17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); $t_{1/2} > 60$ d (Wood et al. 1985; quoted, Olsen & Davis 1990); $k = 0.74$ yr$^{-1}$ with $t_{1/2} = 88–339$ d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24–2.4$ h from air for the reaction with OH radical (USEPA 1974; quoted, Damall et al. 1976);

Photooxidation $t_{1/2} \sim 100$ min for reaction with NO$_2$ under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

photodecomposition $t_{1/2} = 3.0$ h with NO and 3.0 h with NO$_2$ under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 129$ d resulting from the ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2} = 8.0$ d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2} = 286$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes: 130 d for the reaction with NO$_3$ radical for a 12-h nighttime average concn. of $2.4 \times 10^9$ molecule cm$^{-3}$, 12 d for the reaction with OH radical for a 12-h average concn. of $1.0 \times 10^6$ molecule cm$^{-3}$, and > 9.0 yr for the reaction with O$_3$ for a 24-h average concn. of $7 \times 10^{11}$ molecule cm$^{-3}$, (Atkinson et al. 1987).
Surface water: $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k_{\text{exptl}} = (310 \pm 20) \text{ M}^{-1} \text{s}^{-1}$ for direct reaction with ozone in water at pH 2 and 25°C, with $t_{1/2} = 1.80$ min at pH 7 (Yao & Haag 1991).

Ground water: 1344–69000 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation from a ground water field studies of chlorinated ethylenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>Table 5.1.1.28.1</th>
<th>Reported aqueous solubilities of cis-1,2-dichloroethene at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Tse et al. 1992</strong></td>
<td><strong>Wright et al. 1992</strong></td>
</tr>
<tr>
<td>activity coefficient $\gamma_\infty$</td>
<td>activity coefficient $\gamma_\infty$</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
</tr>
<tr>
<td>20</td>
<td>6575</td>
</tr>
<tr>
<td>30</td>
<td>6707</td>
</tr>
<tr>
<td>40</td>
<td>6674</td>
</tr>
<tr>
<td>25</td>
<td>6410</td>
</tr>
<tr>
<td>30</td>
<td>6310</td>
</tr>
<tr>
<td>35</td>
<td>6360</td>
</tr>
<tr>
<td>40</td>
<td>6560</td>
</tr>
</tbody>
</table>

**Figure 5.1.1.28.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cis-1,2-dichloroethene.
**TABLE 5.1.1.28.2**

Reported vapor pressures of *cis*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Ketelaar et al. 1947*163</th>
<th>Flom et al. 1951</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>-58.4</td>
<td>133.3</td>
<td>0.76</td>
</tr>
<tr>
<td>-39.2</td>
<td>666.6</td>
<td>1.68</td>
</tr>
<tr>
<td>-29.9</td>
<td>1333</td>
<td>3.85</td>
</tr>
<tr>
<td>-19.4</td>
<td>2666</td>
<td>6.45</td>
</tr>
<tr>
<td>-7.90</td>
<td>5333</td>
<td>10.73</td>
</tr>
<tr>
<td>-0.50</td>
<td>7999</td>
<td>15.03</td>
</tr>
<tr>
<td>9.50</td>
<td>13332</td>
<td>20.19</td>
</tr>
<tr>
<td>24.6</td>
<td>26664</td>
<td>23.74</td>
</tr>
<tr>
<td>41.0</td>
<td>53329</td>
<td>26.73</td>
</tr>
<tr>
<td>59.0</td>
<td>101325</td>
<td>30.11</td>
</tr>
<tr>
<td>mp/°C</td>
<td>36.35</td>
<td>42823</td>
</tr>
<tr>
<td>-80.5</td>
<td></td>
<td>40.02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45.52</td>
</tr>
<tr>
<td></td>
<td></td>
<td>50.34</td>
</tr>
<tr>
<td></td>
<td></td>
<td>55.28</td>
</tr>
<tr>
<td></td>
<td></td>
<td>59.97</td>
</tr>
<tr>
<td></td>
<td></td>
<td>62.85</td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.56</td>
</tr>
<tr>
<td></td>
<td></td>
<td>71.84</td>
</tr>
<tr>
<td></td>
<td></td>
<td>76.76</td>
</tr>
<tr>
<td></td>
<td></td>
<td>83.63</td>
</tr>
</tbody>
</table>

*for a complete data set, see references.
FIGURE 5.1.1.28.2 Logarithm of vapor pressure versus reciprocal temperature for cis-1,2-dichloroethene.

TABLE 5.1.1.28.3
Reported Henry’s law constants of cis-1,2-dichloroethene at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)
\]

\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)
\]

\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)
\]

\[
\ln \left[ \frac{H}{(\text{Pa} \cdot \text{m}^3/\text{mol})} \right] = A - B/(T/K) \quad (4) \quad \ln \left[ \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right] = A - B/(T/K) \quad (4a)
\]

\[
\ln (k_H/\text{atm} \cdot \text{m}^3/\text{mol}) = A - B/(T/K) + C/(T/K)^2 \quad (5)
\]

Gossett 1987
Ashworth et al. 1988
Tse et al. 1992
Wright et al. 1992

<table>
<thead>
<tr>
<th>EPICS-GC</th>
<th>EPICS-GC</th>
<th>activity coefficient $\gamma^\infty$</th>
<th>activity coefficient $\gamma^\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$H/(\text{Pa} \cdot \text{m}^3/\text{mol})$</td>
<td>$t/°C$</td>
<td>$H/(\text{Pa} \cdot \text{m}^3/\text{mol})$</td>
</tr>
<tr>
<td>10.3</td>
<td>174</td>
<td>10</td>
<td>273.6</td>
</tr>
<tr>
<td>17.5</td>
<td>268.5</td>
<td>15</td>
<td>330.3</td>
</tr>
<tr>
<td>24.8</td>
<td>413.4</td>
<td>20</td>
<td>364.8</td>
</tr>
<tr>
<td>34.6</td>
<td>552</td>
<td>25</td>
<td>460.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>582.6</td>
</tr>
</tbody>
</table>

eq. 4a \quad \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})}

| eq. 4a | A 8.479 | eq. 4a | A 5.164 |
|        | B 4192  |        | B 3143  |
**FIGURE 5.1.1.28.3** Logarithm of Henry's law constant versus reciprocal temperature for cis-1,2-dichloroethene.
5.1.1.29  trans-1,2-Dichloroethene

Common Name: trans-1,2-Dichloroethylene
Synonym: trans-1,2-dichloroethylene, trans-1,2-dichloroethene, trans-acetylene dichloride, Dioform, (E)-1,2-dichloroethene
Chemical Name: trans-1,2-dichloroethylene, trans-1,2-dichloroethene
CAS Registry No: 156-60-5
Molecular Formula: ClCH=CHCl
Molecular Weight: 96.943
Melting Point (°C): –49.8 (Lide 2003)
Boiling Point (°C): 48.7 (Weast 1977, 1982–83)
Density (g/cm³ at 20°C): 1.2565 (Horvath 1982; Weast 1982–83)
Molar Volume (cm³/mol): 77.2 (20°C, calculated-density)
86.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHfus (kJ/mol): 11.98 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
6260 (Seidell 1940)
6300 (selected from literature of measured in DuPont laboratories, McGovern 1943; Dilling 1977)
6260 (recommended, Horvath 1982)
4480, 4480, 4333 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
4488, 4111, 3931 (20, 30, 40°C, activity coeff. γ-differential pressure transducer, Wright et al. 1992)
4488 (20°C, limiting activity coeff. γ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
4520* (tentative values, temp range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
S/(wt%) = 7.803906 – 4.5457 × 10⁻²·(T/K) + 6.96755 × 10⁻⁴·(T/K)², temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
44649* (25.32°C, temp range ~38.19 to 84.84°C, Ketelaar et al. 1947)
43180* (interpolated-Antoine eq. regression, temp range ~65.4 to 47.8°C, Stull 1947)
42970* (25.2°C, dynamic-ebulliometry, measured range 13.5–51.6°C, Flom et al. 1951)
43470 (Hardie 1964)
36743 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 7243.1/(T/K)] + 7.748400; temp range ~65.4 to 236.5°C (Antoine eq., Weast 1972–73)
44190 (calculated-Antoine eq., Boublík et al. 1973)
log (P/mmHg) = 6.96513 – 1141.984/(231.93 + t°C); temp range ~38 to 84°C (Antoine eq. from reported exptl. data, Boublík et al. 1973)
26660, 26660 (14, 20°C, Verschueren 1977, 1983)
40792* (23.138°C, temp range ~0.68 to 46.721°C, Machat 1983; quoted, Boublík et al. 1984)
44190, 43960 (interpolated-Antoine equations, Boublík et al. 1984)
log (P/kPa) = 6.09105 – 1142.553/(231.998 + t/°C); temp range –38.2 to 84.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.04724 – 1112.321/(227.56 + t/°C); temp range –0.68 to 46.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9651 – 1141.9/(231.9 + t/°C); temp range –38.2 to 85°C (Antoine eq., Dean 1985, 1992)

45300 (selected, Riddick et al. 1986)
log (P/kPa) = 6.68147 – 1498.42/(T/K); temp range not specified (Antoine eq., Riddick et al. 1986)

44400 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.93307 – 1059.93/(–50.83 + T/K); temp range 263–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.27465 – 1226.69/(–33.653 + T/K); temp range 321–473 K (Antoine eq.-II, Stephenson & Malanowski 1987)

36250, 53970, 78100 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
log (P/mmHg) = 48.4574 – 3.0496 × 103/(T/K) – 14.694·log (T/K) – 2.1262 × 10–9·(T/K)2; temp range 223–508 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
682.7 (calculated as 1/KAW, Cw/Ca, reported as exptl., Hine & Mookerjee 1975)
1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
669 (calculated-P/C, Dilling 1977)
669 (calculated-P/C, Mackay & Shiu 1981)
950.5 (20°C, EPICS, Lincoff & Gossett 1983; Gossett 1985)
950* (EPICS-GC/FID, measured range 10–34.6°C, Gossett 1987)
ln [H/(atm m3/mol)] = 9.341 – 4182/(T/K); temp range 10.0–34.6°C (EPICS measurements, Gossett 1987)
914 (20°C, EPICS-GC, Yurteri et al. 1987)
539 (gas stripping-GC, Warner et al. 1987)
958* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm-m3/mol)] = 5.333 – 2964/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
729 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
676 (computed value, Yaws et al. 1991)
800, 1196, 1793 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
768.7* (20°C, activity coeff. γ-differential pressure transducer, measured range 20–40°C, Wright et al. 1992)
773 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
634.8 (modified EPICS method-GC, Ryu & Park 1999)
875 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log KAW = 5.247 – 1669/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kow:
2.06 (Hansch & Leo 1985)
2.09 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
2.09 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log koa:

Bioconcentration Factor, log BCF:
1.34 (calculated-Kow, Lyman et al. 1982; quoted, Howard 1990)
1.68 (microorganisms-water, calculated-Kow, Mabey et al. 1982)

Sorption Partition Coefficient, log Koc:
1.56 (calculated-Kow, Lyman et al. 1982; quoted, Howard 1990)
1.77 (sediment-water, calculated-Kow, Mabey et al. 1982)
Environmental Fate Rate Constant, k, and Half-Lives, t½:

Volatileization: experimental t½(exptl) = 24 min for 1 mg/L from water when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982); Evaporation t½(exptl) = 24 min, t½(calc) = 0.85 min, 20.8 min from water (Dilling 1977) Volatilization t½ = 3.0 h from a model river 1 m deep with 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference: kO3 = 3.8 × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984) kOH = 4.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981) kO3 = (1.8 ± 0.29) × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ at 298 K (Zhang et al. 1983) kO3 = 1.2 × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984) kO3 = 2.0 × 10⁻³³ cm² molecule⁻¹ s⁻¹ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984) kO3 = 2.3 × 10⁵ cm³ mol⁻¹ s⁻¹, estimated at 300 K (Lyman 1982) k < 10⁸ M⁻¹ h⁻¹ for singlet oxygen and 6.0 M⁻¹ h⁻¹ for peroxy radicals at 25°C (Mabey et al. 1982) k = (5.7 ± 1.0) × 10⁵ M⁻¹ s⁻¹ for the reaction with ozone in water using 1 mM t-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983) kO3 = 1.8 × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ at room temp. (Tuazon et al. 1984) kOH = 1.79 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1986; quoted, Atkinson et al. 1987; Sabljic & Güsten 1990) kNO3 = 5.7 ± 2.7)5 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Atkinson et al. 1987) kNO3 = 5.7 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ with a calculated atmospheric lifetime of 179 d, kOH = 1.8 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a lifetime of 5.1 d and kO3 = 1.5 × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ with a lifetime of 110 d at room temp. (Atkinson et al. 1987) kOH(calc) = 2.5 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, kOH(obs.) = 1.8 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1987) photooxidation t½ = 25.2 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991) kNO3 = 1.11 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990) kNO3 = (1.07 ± 0.11) × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ relative to ethene at 298 ± 2 K (Atkinson 1991) kOH(calc) = 2.57 × 10⁻¹³ cm² molecule⁻¹ s⁻¹ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis:

Biodegradation: aqueous aerobic t½ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic t½ = 2688–17280 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991); k = 0.1 yr⁻¹ with t½ = 53 d (Wood et al. 1985; quoted, Olsen & Davis 1990); rate constant k = 0.12–0.35 mini⁻¹ in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989); k = 1.8 yr⁻¹ with t½ = 132–147 d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance t½ = 0.24–2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); photodecomposition t½ = 2.9 h with NO and t½ = 2.8 h with NO2 under simulated atmospheric conditions (Dilling et al. 1976); Photooxidation t½s ~ 100 min for reaction with NO2 under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)
residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

t$_{1/2}$ = 44 d resulting from ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

t$_{1/2}$ = 3.6 d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

t$_{1/2}$ = 25.2 h, based on estimated rate constant for reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes, $\tau$ = 170 d for the reaction with NO$_3$ radical for a 12-h nighttime average concn. of $2.4 \times 10^6$ molecule·cm$^{-3}$, $\tau$ = 5.1 d for the reaction with OH radical for a 12-h average concn. of $1.0 \times 10^6$ molecule·cm$^{-3}$, and $\tau$ = 110 d for the reaction with O$_3$ for a 24-h average concentration of $7 \times 10^{11}$ molecule·cm$^{-3}$ (Atkinson et al. 1987).

Surface water: t$_{1/2}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: t$_{1/2}$ = 1344–69000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and estimated half-life for anaerobic biodegradation of chlorinated ethylenes from a ground water field study (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: t$_{1/2}$ = 672–4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$\tau$ < 10 d (Ryan et al. 1988).

Biota: t$_{1/2}$ < 10 d, subject to plant uptake via volatilization (Ryan et al. 1988).

---

**TABLE 5.1.1.29.1**

Reported aqueous solubilities of trans-1,2-dichloroethene at various temperatures

<table>
<thead>
<tr>
<th>Tse et al. 1992</th>
<th>Wright et al. 1992</th>
<th>Horvath &amp; Getzen 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>activity coefficient $\gamma^a$</td>
<td>activity coefficient $\gamma^a$</td>
<td>IUPAC-NIST recommended</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m$^{-3}$</td>
<td>t/°C</td>
</tr>
<tr>
<td>20</td>
<td>4480</td>
<td>20</td>
</tr>
<tr>
<td>30</td>
<td>4480</td>
<td>30</td>
</tr>
<tr>
<td>40</td>
<td>4333</td>
<td>40</td>
</tr>
<tr>
<td>25</td>
<td>4520</td>
<td>30</td>
</tr>
<tr>
<td>35</td>
<td>4190</td>
<td>35</td>
</tr>
<tr>
<td>40</td>
<td>4080</td>
<td>40</td>
</tr>
</tbody>
</table>
**TABLE 5.1.1.29.2**

Reported vapor pressures of *trans*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th></th>
<th>Log P = A – B/(T/K)</th>
<th>ln P = A – B/(T/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ln P = A – B/(C + t/°C)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>log P = A – B/(C + T/K)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>log P = A – B/(T/K) – C·log (T/K)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–65.4</td>
<td>133.3</td>
<td>–38.19</td>
<td>1387</td>
<td>13.5</td>
<td>26131</td>
<td>–0.68</td>
<td>13944</td>
</tr>
<tr>
<td>–47.4</td>
<td>666.6</td>
<td>–28.3</td>
<td>3000</td>
<td>20.5</td>
<td>35210</td>
<td>3.154</td>
<td>16825</td>
</tr>
<tr>
<td>–38.0</td>
<td>1333</td>
<td>–15.12</td>
<td>6733</td>
<td>25.3</td>
<td>42956</td>
<td>7.12</td>
<td>20300</td>
</tr>
<tr>
<td>–28.0</td>
<td>2666</td>
<td>–7.29</td>
<td>10092</td>
<td>29.7</td>
<td>50836</td>
<td>11.306</td>
<td>24599</td>
</tr>
<tr>
<td>–17.0</td>
<td>5333</td>
<td>0.52</td>
<td>15086</td>
<td>34.7</td>
<td>61835</td>
<td>15.344</td>
<td>29372</td>
</tr>
<tr>
<td>–10.0</td>
<td>7999</td>
<td>5.98</td>
<td>19438</td>
<td>38.6</td>
<td>71581</td>
<td>19.302</td>
<td>34777</td>
</tr>
<tr>
<td>–0.20</td>
<td>13332</td>
<td>11.12</td>
<td>24718</td>
<td>41.6</td>
<td>79300</td>
<td>23.138</td>
<td>40792</td>
</tr>
<tr>
<td>14.3</td>
<td>26664</td>
<td>16.91</td>
<td>31651</td>
<td>44.1</td>
<td>86513</td>
<td>27.017</td>
<td>47616</td>
</tr>
<tr>
<td>30.8</td>
<td>53329</td>
<td>19.06</td>
<td>34757</td>
<td>46.8</td>
<td>95099</td>
<td>33.103</td>
<td>60215</td>
</tr>
<tr>
<td>47.8</td>
<td>101325</td>
<td>25.32</td>
<td>44649</td>
<td>49.1</td>
<td>102165</td>
<td>38.951</td>
<td>74768</td>
</tr>
<tr>
<td></td>
<td></td>
<td>28.23</td>
<td>50329</td>
<td>51.6</td>
<td>111151</td>
<td>45.27</td>
<td>93376</td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.29.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *trans*-1,2-dichloroethene.
TABLE 5.1.1.29.2 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>mp/°C</td>
<td>–122.5</td>
<td>32.15</td>
<td>38448</td>
<td>46.72</td>
<td>98149</td>
<td>43.72</td>
<td>88272</td>
</tr>
<tr>
<td>35.84</td>
<td>66888</td>
<td>ΔHv/(kJ mol⁻¹) = 29.62</td>
<td>bp/°C</td>
<td>47.655</td>
<td>Antoine eq</td>
<td></td>
<td></td>
</tr>
<tr>
<td>47.17</td>
<td>99365</td>
<td></td>
<td>eq. 2</td>
<td>P/kPa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>48.83</td>
<td>105591</td>
<td>A</td>
<td>6.04724</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50.82</td>
<td>112737</td>
<td>B</td>
<td>1112.321</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m.p.</td>
<td>–49.8 °C</td>
<td>56.12</td>
<td>133389</td>
<td>63.58</td>
<td>167812</td>
<td>68.19</td>
<td>192917</td>
</tr>
<tr>
<td>77.16</td>
<td>248619</td>
<td>84.84</td>
<td>304561</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*for a complete data set, see references.

FIGURE 5.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for trans-1,2-dichloroethene.
### TABLE 5.1.1.29.3
Reported Henry’s law constants of *trans*-1,2-dichloroethene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Units</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ln K_{AW} = A - B/(T/K) )</td>
<td>( \text{log K}_{AW} = A - B/(T/K) )</td>
<td>(1)</td>
</tr>
<tr>
<td>( \ln (1/K_{AW}) = A - B/(T/K) )</td>
<td>( \log (1/K_{AW}) = A - B/(T/K) )</td>
<td>(2)</td>
</tr>
<tr>
<td>( \ln (k_H/\text{atm}) = A - B/(T/K) )</td>
<td>( \log (k_H/\text{atm}) = A - B/(T/K) )</td>
<td>(3)</td>
</tr>
<tr>
<td>( \ln \left[ H/(\text{Pa m}^3/\text{mol}) \right] = A - B/(T/K) )</td>
<td>( \log \left[ H/(\text{atm m}^3/\text{mol}) \right] = A - B/(T/K) )</td>
<td>(4)</td>
</tr>
<tr>
<td>( K_{AW} = A - B(T/K) + C(T/K)^2 )</td>
<td>( \ln \left[ H/(\text{atm m}^3/\text{mol}) \right] = A - B/(T/K) )</td>
<td>(5)</td>
</tr>
</tbody>
</table>

#### Reported Henry’s law constants of *trans*-1,2-dichloroethene at various temperatures

<table>
<thead>
<tr>
<th>EPICS-GC</th>
<th>EPICS-GC</th>
<th>EPICS-GC</th>
<th>EPICS-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/\degree C )</td>
<td>( H/(\text{Pa m}^3/\text{mol}) )</td>
<td>( t/\degree C )</td>
<td>( H/(\text{Pa m}^3/\text{mol}) )</td>
</tr>
<tr>
<td>10.0</td>
<td>425.6</td>
<td>10</td>
<td>597.8</td>
</tr>
<tr>
<td>17.5</td>
<td>668.7</td>
<td>15</td>
<td>714.3</td>
</tr>
<tr>
<td>24.8</td>
<td>950.4</td>
<td>20</td>
<td>868.4</td>
</tr>
<tr>
<td>34.6</td>
<td>1398.3</td>
<td>25</td>
<td>957.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>1226.0</td>
</tr>
</tbody>
</table>

#### Equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Units</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ln \left[ H/(\text{atm m}^3/\text{mol}) \right] = A - B/(T/K) )</td>
<td>( \log \left[ H/(\text{atm m}^3/\text{mol}) \right] = A - B/(T/K) )</td>
<td>(4a)</td>
</tr>
</tbody>
</table>

#### Henry’s law constant vs. 1/T

**FIGURE 5.1.1.29.3** Logarithm of Henry’s law constant versus reciprocal temperature for *trans*-1,2-dichloroethene.
5.1.1.30 Trichloroethylene

Chemical Name: 1,1,2-trichloroethylene
CAS Registry No: 79-01-6
Molecular Formula: C₂HCl₃, CHCl=CCl₂
Molecular Weight: 131.388
Melting Point (°C):
\[ -84.7 \quad \text{(Lide 2003)} \]
Boiling Point (°C):
\[ 87.21 \quad \text{(Lide 2003)} \]
Density (gm/cm³ at 20°C):
\[ 1.4642 \quad \text{(Dreisbach 1959; Horvath 1982; Weast 1982–83)} \]
\[ 1.4554 \quad \text{(25°C, Dreisbach 1959)} \]
Molar Volume (cm³/mol):
\[ 89.02 \quad \text{(calculated-density, Miller et al. 1985)} \]
\[ 107.1 \quad \text{(calculated-Le Bas method at normal boiling point)} \]
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
\[ 34.27, 31.47 \quad \text{(25°C, bp, Riddick et al. 1986)} \]
Enthalpy of Fusion, \( \Delta H_{ fus } \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{ fus } \) (J/mol K):
Fugacity Ratio at 25°C, \( F \): 1.0 (Suntio et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
\[ 1818 \quad \text{(volumetric method, Wright & Schaffer 1932;)} \]
\[ 1100 \quad \text{(data presented in graph, temp range 0–80°C, McGovern 1943)} \]
\[ 1288^* \quad \text{(temp range 10–50°C, Valraud et al. 1957)} \]
\[ 1100 \quad \text{(20°C, McConnell et al. 1975; Pearson & McConnell 1975)} \]
\[ 1780, 1500, 1470 \quad \text{(3, 20, 34°C, shake flask-GC/ECD, Chiou & Freed 1977)} \]
\[ 1000, 1100, 1100 \quad \text{(1.5, 20, 25°C, literature average, Dilling 1977)} \]
\[ 1000 \quad \text{(shake flask-titration/turbidity, Coca et al. 1980)} \]
\[ 1472 \quad \text{(shake flask-LSC, Banerjee et al. 1980)} \]
\[ 1474 \quad \text{(shake flask-LSC, Veith et al. 1980)} \]
\[ 1100^* \quad \text{(summary of literature data, temp range 0–80°C, Horvath 1982)} \]
\[ 1366 \quad \text{(generator column-HPLC, Tewari et al. 1982)} \]
\[ 743.1 \quad \text{(30°C, headspace-GC, McNally & Grob 1984)} \]
\[ 1370 \quad \text{(selected, Riddick et al. 1986)} \]
\[ 1421 \quad \text{(23–24°C, shake flask-GC, Broholm et al. 1992)} \]
\[ 1350 \quad \text{(20°C, calculated-activity coefficients, Wright et al. 1992)} \]
\[ 1483, 1450, 1468 \quad \text{(20, 30, 40°C, infinite dilution activity coeff. \( \gamma \)-GC, Tse et al. 1992)} \]
\[ 1349, 1409, 1308 \quad \text{(20, 30, 40°C, activity coeff. \( \gamma \)-differential pressure transducer, Wright et al. 1992)} \]
\[ 1300–1500 \quad \text{(9–71°C, generator column-GC, data presented in graph, Heron et al. 1998)} \]
\[ 1330 \quad \text{(20°C, limiting activity coeff. \( \gamma \) by equilibrium air stripping-GC, Hovorka & Dohnal 1997)} \]
\[ 1280^* \quad \text{(recommended, temp range 0–60°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)} \]
\[ S/(wt\%) = 1.4049 – 8.2223 \times 10^{-3} \times (T/K) + 1.3218 \times 10^{-5} \times (T/K)^2, \quad \text{temp range 273–333 K (equation derived from literature solubility data, Horvath & Getzen 1999a)} \]
\[ 1417^* \quad \text{(21°C, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range 21–117°C, Knauss et al. 2000)} \]
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19733* (temp range 25–87.15°C, Hertz & Rathmann 1912)
9331 (extrapolated, data presented in graph, McGovern 1943)
9645* (25.5°C, ebulliometry, measured range 18–86°C, McDonald 1944)

\[
\begin{align*}
\log (P/\text{cmHg}) &= 30.482609 – 2936.227/(T/K) – 7.999975 \cdot \log (T/K); \text{ temp range 18–86°C (ebulliometry, McDonald 1944)} \\
9735* \text{ (interpolated-Antoine eq. regression, temp range 25–87.2°C, Stull 1947)} \\
9906 \text{ (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)} \\
&\log (P/\text{mmHg}) = 7.02808 – 1315.0/(230.0 + t/°C); \text{ temp range 7–155°C (Antoine eq. for liquid state, Dreisbach 1959)} \\
9723 \text{ (calculated-Antoine eq., Weast 1972–73)} \\
&\log (P/\text{mmHg}) = [–0.2185 \times 8314.7/(T/K)] + 7.956342; \text{ temp range } –43.8 \text{ to 86.7°C (Antoine eq., Weast 1972–73)} \\
9224 \text{ (calculated-Antoine eq., Boublik et al. 1973)} \\
&\log (P/\text{mmHg}) = 6.51827 – 1018.603/(192.731 + t/°C); \text{ temp range 17–86°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)} \\
8000 \text{ (20°C, Perry & Chilton 1973)} \\
7700 \text{ (20°C, McConnell et al. 1975; Pearson & McConnell 1975)} \\
3066, 7866, 9866 \text{ (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)} \\
7998, 12660 \text{ (20°C, 30°C, Verschueren 1983; Hewitt et al. 1992)} \\
9200, 9690 \text{ (interpolated-Antoine equations., Boublik et al. 1984)} \\
&\log (P/\text{kPa}) = 5.59553 – 994.46/(189.705 + t/°C); \text{ temp range 17.8–86.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \\
9723 \text{ (calculated-Antoine eq., Weast 1972–73)} \\
&\log (P/\text{kPa}) = 6.15298 – 1315.0/(230.0 + t/°C); \text{ temp range 7–155°C (Antoine eq. for liquid state, Weast 1972–73)} \\
9906 \text{ (calculated-Antoine eq., Weast 1972–73)} \\
&\log (P/\text{mmHg}) = 6.5183 – 1018.6/(192.7 + t/°C); \text{ temp range 18–86°C (Antoine eq. from reported exptl. data, Dean 1985, 1992)} \\
6307 (selected, Riddick et al. 1986) \\
&\log (P/\text{kPa}) = 6.15298 – 1315.04/(–43.15 + T/K); \text{ temp range 280–428 K (vapor pressure eq., Yaws 1994)} \\
9691 \text{ (resistance measurement-Antoine eq., Foco et al. 1992)} \\
7753, 12350, 19080 \text{ (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)} \\
&\log (P/\text{mmHg}) = 23.6735 – 2.3763 \times 10^3/(T/K) – 5.8275 \cdot \log (T/K) + 1.9586 \times 10^{-3} \cdot (T/K) + 2.8882 \times 10^{-14} \cdot (T/K)^2; \text{ temp range 188–571 K (vapor pressure eq., Yaws 1994)} \\

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1186 (calculated as 1/K_\text{AW}, C_\text{w}/C_\text{x}, reported as exptl., Hine & Mookerjee 1975)
248, 1186 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
967 (calculated-P/C, Neely 1975)
388.2, 1215 (1.5, 25°C, calculated-P/C, Dilling 1977)
890, 975 (20°C, exptl., calculated-P/C, Dilling 1977)
1103 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

\[
\begin{align*}
\log (H/\text{atm}) &= 8.59 – 1716.16/(T/K) \text{ (least-square regression of data from lit., Kavanaugh & Trussell 1980)} \\
985 \text{ (20°C, batch stripping-GC, Mackay et al. 1979)} \\
985* \text{ (25.2°C, equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)} \\
\ln (k_{\text{H}}/\text{atm}) &= 21.89 – 4647/(T/K); \text{ temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)} \\
999 \text{ (20°C, batch stripping-GC, Munz & Roberts 1987)} \\
970 \text{ (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)} \\
774; 683 \text{ (20°C, EPICS-GC; batch air stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)} \\
\ln [H/(\text{atm m}^3/\text{mol})] &= 11.94 – 4929/(T/K); \text{ temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)} \\
\ln [H/(\text{atm m}^3/\text{mol})] &= 9.703 – 4308/(T/K); \text{ temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)}
\end{align*}
\]
Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.37 (Hansch & Elkins 1971)
2.29 (Leo et al. 1971; Hansch & Leo 1979; 1987)
2.61 (shake flask-GC/ECD, Chiu & Freed 1977)
2.42 (shake flask-LSC, Banerjee et al. 1980)
2.42 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982; Veith et al. 1983)
2.86 (HPLC-k’ correlation, McDuffie 1981)

© 2006 by Taylor & Francis Group, LLC
Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:
2.99  (calculated-measured infinite dilution activity coeff. and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:
- 1.59  (rainbow trout, Neely et al. 1974)
- 1.23–1.36  (calculated-$K_{OW}$, Veith et al. 1979; Veith et al. 1980)
- 1.23  (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 1.23–1.59  (bluegill sunfish & rainbow trout, Barrows et al. 1980; Lyman 1981)
- 1.59  (rainbow trout, quoted, Bysshe 1982)
- 1.987  (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)
- 1.20  (calculated-MCI $\chi$, Koch 1983)
- 2.996  (activated sludge, Freitag et al. 1984)
- 3.06, 2.39  (Chlorella fusca, calculated-$K_{OW}$, Geyer et al. 1984)
- 1.20, 1.05  (quoted, calculated, Subljic 1987)
- 1.025  (quoted from USEPA 1986, Yeh & Kastenberg 1991)
- 1.420  (calculated-$K_{OW}$, McCarty et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:
- 2.10  (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
- 2.20  (Pavlou & Weston 1983, 1984)
- 1.76, 2.20  (ICN humic acid-coated $Al_2O_3$, ICN humic acid, Garbarini & Lion 1985)
- 1.66; 2.14, 2.40  (predicted-$S$, predicted-$K_{OW}$, Garbarini & Lion 1985)
- 1.76; 0.616  (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, Garbarini & Lion 1986)
- 1.238, 2.079, 2.045, 0.30, 1.827  (tannic acid, lignin, zein, cellulose, Aldrich humic acid, Garbarini & Lion 1986)
- 2.025, 2.086  (Sapsucker Woods soil, Sapsucker Woods ether-extracted soil, Garbarini & Lion 1986)
- 2.161, 2.458  (humin, oxidized humin, Garbarini & Lion 1986)
- 2.663  (fats, waxes, resins, Garbarini & Lion 1986)
- 2.54, 1.72  (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
- 2.00; 1.84  (quoted from Seip et al. 1986, calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 2.03  (soil, Chiou et al. 1988; quoted, Grathwohl 1990)
- 2.02, 2.11  (soil: quoted, HPLC-RT correlation, Hodson & Williams 1988)
- 1.79  (20°C, humic acid, Peterson et al. 1988; quoted, Grathwohl 1990)
- 1.53  (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.61, 2.12  (organic cations treated Marlette soil A horizon; HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.89, 2.50, 2.25  (organic cations treated Marlette soil B horizon; HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.09; 2.56; 3.43  (20°C, soil, sand and loess; weathered shale and mudrock; unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 1.97, 2.15  (20°C, calculated-$K_{OW}$, Grathwohl 1990)
- 0.30–3.64  (cellulose anthracite, quoted, Grathwohl 1990)
- 2.01  (calculated average, Olsen & Davis 1990)
- 2.20, 1.78  (humic acid, humic acid-coated $Al_2O_3$, Pavlostathis & Jaglal 1991)
- 2.03  (surface soil, Pavlostathis & Jaglal 1991)
Halogenated Aliphatic Hydrocarbons

3.39, 2.00 (organic carbon soil, Doust & Huang 1992)
1.60, 1.60, 2.15 (bentonite, green & tan clay, Doust & Huang 1992)
0.35, 1.40, 1.90, 2.20 (Barnwell, Congaree, McBean I & II sands, Doust & Huang 1992)
1.66, 2.64, 2.83 (calculated-equilibrium desorption data, Pavlostathis & Mathavan 1992)
2.23, 2.33, 2.35, 2.34, 2.36, 2.41 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon fOC = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
2.80; 2.00 (soil, calculated-universal solvation model; quoted exper., Winget et al. 2000)
1.92, 2.00, 1.75 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%; average, Delle Site 2001)

Sorption Partition Coefficient, log KOM:
1.23 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.42, 1.89 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.78, 2.36 (organic cations treated Marlette soil Bt horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil Bt horizon OM 4.38%; Oshtemo soil Bt horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.74 (Florida peat, OC 57.1%, batch equilibrium-sorption isotherm, Rutherford & Chiou 1992)

Environment Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: evaporation t½(exptl.) = 21 min, calculated t½(calc) = 0.48 min from dilute aqueous solution of 1 ppm initial concn. in a 250 mL beaker with constant stirring at room temp (Dilling et al. 1975);
vaporization k = 2.79, 5.07 g cm⁻² s⁻¹ at 23.7 ± 0.5°C into the atmosphere (Choi & Freed 1977);
Evaporation t½(exptl.) = 17.7, 18.5, 23.5 min, t½(calc) = 0.47 min, 23.8 min at 20–25°C and 1.5°C from water (Dilling 1977)
the ratio of evaporation rate constant to that of oxygen reaeration rate constant: measured as 0.49 as compared to the predicted 0.44 (Smith et al. 1980);
t½(exptl.) = 1.42 × 10⁴ s and t½(calc) = 5.1 × 10³ s for water body of depth of 22.5 m (Klöpffer et al. 1982)
estimated t½ = 3.4 h from water (Thomas 1982);
k = 0.025 d⁻¹, t½ = 28 d in spring at 8–16°C, k = 0.052 d⁻¹, t½ = 13 d in summer at 20–22°C, k = 0.045 d⁻¹,
t½ = 15 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.064 d⁻¹,
t½ = 10.7 d with HgCl₂, and k = 0.081 d⁻¹, t½ = 9.6 d without HgCl₂ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);
k = 7.22 × 10⁻¹ h⁻¹ (Mackay et al. 1985).

Photolysis:
t½ = 3.5 h estimated from lab. simulated UV photolysis (light intensity about 6 times of natural sunlight at noon on a summer day in Freeport) for 10 ppm to react with 5 ppm NO at 27 ± 1°C (Dilling et al. 1976); probably would not occur (Callahan et al., 1979)
photocatalyzed mineralization by the presence of TiO₂ with the rate of 830 ppm min⁻¹ g⁻¹ of catalyst (Ollis 1985);
k = (4.08–6.27) × 10⁻³ h⁻¹ with H₂O₂ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation:
rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kO₃ with NO, Oxidation with NO, with O₃ and/or the Arrhenius expression see reference:
kOH = 2.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (discharge flow system-LMR, Howard 1976)
Photooxidation t½ = 120 min for reaction with NO, under UV irradiation (Gay, Jr. et al. 1976)
kOH * = (2.37 ± 0.1) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K, measured range 234–420 K (discharge flow-resonance fluorescence, Chang & Kaufman 1977)
kOH = (0.27 ± 0.08) × 10¹⁰ cm³ M⁻¹ s⁻¹ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1978)
kOH = 2.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson et al. 1979,1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)
kOH = 0.22 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ estimated, and kO₃ = 3.6 × 10³ cm³ mol⁻¹ s⁻¹ at 300 K by urban environments (Singh et al. 1980)
kOH = 1.2 × 10⁻¹² cm³ mol⁻¹ s⁻¹ estimated, and kO₃ = 3.6 × 10³ cm³ mol⁻¹ s⁻¹ at 300 K (Lyman 1982)
k_{O3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the gas-phase reaction with ozone at } 296 \pm 2 \text{ K (Atkinson et al. 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)}

k < 1000 \text{ M}^{-1} \text{ h}^{-1} \text{ for singlet oxygen, } k = 6.0 \text{ M}^{-1} \text{ h}^{-1} \text{ for RO}_2 \text{ radical (Mabey et al. 1982)}

k = (17 \pm 4) \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)}

k_{O3} = 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ } k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Tuazon et al. 1984)}

k_{OH}^{(calc)} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ } k_{OH}^{(obs.)} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR [structure-activity relationship], Atkinson 1985)}

k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.10 \text{ d}^{-1}, k_{O3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.002 \text{ d}^{-1} \text{ at room temp. (Atkinson et al. 1985)}

k_{OH} = (2.86 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with reference to n-butane at } 23.2 \pm 1.1°C \text{ and a calculated atmospheric lifetime } \tau = 4.0 \text{ d (Edney et al. 1986)}

k_{O3} = (1.5 \pm 0.7) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 2 \text{ K (relative rate method, Atkinson et al. 1987)}

k_{O3} = 1.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated atmospheric lifetime } \tau = 64 \text{ d, } k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with lifetime } \tau = 9.6 \text{ d and } k_{O3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with lifetime } \tau > 1.5 \text{ yr at room temp. (Atkinson et al. 1987)}

k_{OH}^{(calc)} = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ } k_{OH}^{(obs.)} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR [structure-activity relationship], Atkinson 1987)}

k_{OH}^{*} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)}

k_{OH}^{(calc)} = 6.92 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (as per Atkinson 1987 and 1988, Müller & Klein 1991)}

k_{O3} = (2.81 \pm 0.17) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ relative to ethene at } 298 \pm 2 \text{ K (Atkinson 1991)}

k^{(aq.)} = (15 \pm 2) \text{ M}^{-3} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 2 and 21 \pm 1°C, with a half-life of 37 min at pH 7 (Yao & Haag 1991)}.

Hydrolysis: not an important process (Mabey et al. 1982);

k = 0.065 \text{ month}^{-1} \text{ at } 25°C \text{ with } t_{1/2} = 10.7 \text{ months (Dilling et al. 1975; quoted, Howard et al. 1991)};

k = 9.0 \times 10^{-5} \text{ h}^{-1} \text{ (Mackay et al. 1985)};

abiomic hydrolysis or dehydrohalogenation \text{ } t_{1/2} = 10.7 \text{ months (Olsen & Davis 1990)}

\text{ } t_{1/2} = 320 \text{ d at pH 7 in natural waters (Capel & Larson 1995)}

Biodegradation: can be biodegraded by microorganisms in sea water;

\text{ } t_{1/2}(\text{aerobic}) = 6 \text{ months to } 1 \text{ yr based on acclimated soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991)};

k = 1.1 \text{ yr}^{-1} \text{ with } t_{1/2} = 230 \text{ d (Roberts et al. 1982; quoted, Olsen & Davis 1990)}

\text{ } t_{1/2}(\text{anaerobic}) = 98 \text{ d based on sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991)};

k = 0.06 \text{ yr}^{-1} \text{ with biodegradation } t_{1/2} = 33 \text{ d, microcosm constructed with crushed rock and water containing low microbial biomass depleted all TCE in } 21 \text{ months of incubation (Barrio-Lage et al. 1987, quoted, Olsen & Davis 1990)}

k \sim 0.02 \text{ min}^{-1} \text{ in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989)};

k = 0.08 \text{ yr}^{-1} \text{ with } t_{1/2} = 43 \text{ d (Olsen & Davis 1990)}

\text{ } t_{1/2}(\text{aerobic}) = 180 \text{ d, } t_{1/2}(\text{anaerobic}) = 98 \text{ d in natural waters (Capel & Larson 1995)}

Biotransformation: estimated rate constant of } 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1} \text{ for bacteria (Mabey et al. 1982)}.

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

k_1 = 10.5 \text{ h}^{-1} \text{ (flagfish, calculated-BCF } \times k_2, \text{ McCarty et al. 1992)}

k_2 = 0.398 \text{ h}^{-1} \text{ (flagfish, estimated-one compartment first-order kinetics, McCarty et al. 1992)}

Environmental Half-Lives:

Air: tropospheric \text{ } t_{1/2} = 6.0 \text{ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)}

\text{ } \text{disappearance } t_{1/2} = 0.24–2.4 \text{ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnell et al. 1976)};

\text{ } \text{photodecomposition } t_{1/2} = 3.5 \text{ h with NO and } t_{1/2} = 2.9 \text{ h with NO}_2 \text{ under simulated atmospheric conditions (Dilling et al. 1976)};

\text{ } \text{photooxidation } t_{1/2} \sim 120 \text{ min for reaction with NO}_2 \text{ under UV irradiation (Gay, Jr. et al. 1976)}

\text{ } \text{residence time of } 5.3 \text{ d, loss of } 17.2\% \text{ in } 1 \text{ d or } 12 \text{ sunlit hours at } 300 \text{ K in urban environments (Singh et al. 1981)}
Halogenated Aliphatic Hydrocarbons

\[ t_{1/2} = 27–272 \text{ h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);} \]

atmospheric lifetime \( \tau = 4.0 \text{ d, based on the photooxidation rate constant in the gas phase at} \]
\[ 23.2 \pm 1.1^\circ \text{C (Edney et al. 1986);} \]

atmospheric lifetimes \( \tau = 64 \text{ d for the reaction with NO}_3 \text{ for a 12-h nighttime average concn. of} \]
\[ 2.4 \times 10^9 \text{ molecule/cm}^3, \tau = 9.6 \text{ d for the reaction with OH radical for a 12-h average concn. of} \]
\[ 1.0 \times 10^4 \text{ molecule cm}^{-3}, \text{ and } \tau > 1.5 \text{ yr for the reaction with O}_3 \text{ for a 24-h average concn. of} \]
\[ 7 \times 10^{11} \text{ molecule/cm}^3 \]
(Atkinson et al. 1987);

\[ t_{1/2} \sim 3.7 \text{ d (Yeh & Kastenberg 1991).} \]

Surface water: estimated \( t_{1/2} = 1.2–90 \text{ d in surface waters at various locations in the Netherlands in case of a first} \]
order reduction process (Zoeteman et al. 1980)

half-lives from marine mesocosm: \( t_{1/2} = 28 \text{ d in the spring at 8–16^\circ \text{C,} t_{1/2} = 13 \text{ d in the summer at 20–22^\circ \text{C}} \]
and \( t_{1/2} = 15 \text{ d in the winter at 3–7^\circ \text{C when volatilization dominates, and} t_{1/2} = 10.7 \text{ d and 8.6 d for} \]
experiments with and without HgCl}_2 as poison, respectively, in September 9–15 (Wakeham et al. 1983)

Biodegradation \( t_{1/2} \text{(aerobic)} = 100 \text{ d,} t_{1/2} \text{(anaerobic)} = 400 \text{ d; hydrolysis} t_{1/2} = 320 \text{ d at pH 7 in natural waters} \]
(Capel & Larson 1995)

\[ t_{1/2} = 4320–8640 \text{ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)} \]
\[ t_{1/2} \sim 90 \text{ d (Yeh & Kastenberg 1991);} \]

measured rate constant \( k = (15 \pm 2) \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 2 and 21 \pm 1^\circ \text{C},} \]
with \( t_{1/2} = 37 \text{ min at pH 7 (Yao & Haag 1991).} \]

Ground water: \( t_{1/2} = 7704–39672 \text{ h, based on hydrolysis half-life (Dilling et al. 1975; quoted, Howard et al. 1991)} \]
and anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991)

\[ t_{1/2} \sim 2.0 \text{ yr in the ground water in the Netherlands (estimated, Zoeteman et al. 1981);} \]
\[ t_{1/2} \sim 86 \text{ d (Yeh & Kastenberg 1991).} \]

Soil: \( t_{1/2} < 10 \text{ d (Ryan et al. 1988);} \]

\[ t_{1/2} = 4320–8640 \text{ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)} \]
\[ t_{1/2} \sim 43 \text{ d in upper soil and} t_{1/2} \sim 86 \text{ d in lower soil (Yeh & Kastenberg 1991).} \]

Sediment: \( t_{1/2} \sim 43 \text{ d (estimated, Yeh & Kastenberg 1991).} \]

Biota: \( t_{1/2} < 1 \text{ d in tissues of bluegill sunfish (Barrows et al. 1980);} \]

\[ t_{1/2} < 10 \text{ d, subject to plant uptake via volatilization (Ryan et al. 1988).} \]

**TABLE 5.1.1.30.1**

Reported aqueous solubilities of trichloroethylene at various temperatures

\[
\begin{align*}
S/(\text{wt}) = 0.10494 + 4.9038 \times 10^{-5} \cdot (t/\text{°C}) + 6.4541 \times 10^{-6} \cdot (t/\text{°C})^2 - 1.8808 \times 10^{-8} \cdot (t/\text{°C})^3 & \quad (1) \\
S/(\text{wt}) = 1.4049 - 8.2223 \times 10^{-3} \cdot (T/\text{K}) + 1.3218 \times 10^{-5} \cdot (T/\text{K})^2 & \quad (2)
\end{align*}
\]

1. Vallaud et al. 1957

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1280</td>
<td>0</td>
<td>1049</td>
<td>20</td>
<td>1061</td>
<td>30</td>
<td>1099</td>
</tr>
<tr>
<td>20</td>
<td>1285</td>
<td>10</td>
<td>1061</td>
<td>25</td>
<td>1083</td>
<td>40</td>
<td>1117</td>
</tr>
<tr>
<td>25</td>
<td>1288</td>
<td>20</td>
<td>1083</td>
<td>30</td>
<td>1117</td>
<td>50</td>
<td>1160</td>
</tr>
<tr>
<td>30</td>
<td>1290</td>
<td>25</td>
<td>1099</td>
<td>40</td>
<td>1160</td>
<td>50</td>
<td>1212</td>
</tr>
<tr>
<td>40</td>
<td>1305</td>
<td>30</td>
<td>1117</td>
<td>60</td>
<td>1271</td>
<td>70</td>
<td>1335</td>
</tr>
<tr>
<td>50</td>
<td>1330</td>
<td>40</td>
<td>1160</td>
<td>80</td>
<td>1405</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
TABLE 5.1.1.30.1 (Continued)

2. 

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1450</td>
<td>40</td>
<td>1260</td>
</tr>
<tr>
<td>5</td>
<td>1410</td>
<td>45</td>
<td>1270</td>
</tr>
<tr>
<td>10</td>
<td>1370</td>
<td>50</td>
<td>1280</td>
</tr>
<tr>
<td>15</td>
<td>1330</td>
<td>55</td>
<td>1300</td>
</tr>
<tr>
<td>20</td>
<td>1310</td>
<td>60</td>
<td>1330</td>
</tr>
<tr>
<td>25</td>
<td>1280</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1279</td>
<td>eq. 2</td>
<td>S/wt%</td>
</tr>
<tr>
<td>35</td>
<td>1260</td>
<td>temp range 273–333 K</td>
<td></td>
</tr>
</tbody>
</table>

Horvath & Getzen 1999a

summary of literature data

Knauss et al. 2000

batch equilibrium-GC

at 1.0 MPa

t/°C S/g·m⁻³ t/°C S/g·m⁻³
21 1417
50 1450
75 1878
99 2872
117 5268

FIGURE 5.1.1.30.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for trichloroethylene.
## TABLE 5.1.1.30.2
Reported vapor pressures of trichloroethylene at various temperatures and the coefficients for the vapor pressure equations

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \log P = A - B/(T/K) )</td>
<td>( \ln P = A - B/(T/K) )</td>
</tr>
<tr>
<td></td>
<td>( \log P = A - B/(C + t/°C) )</td>
<td>( \ln P = A - B/(C + t/°C) )</td>
</tr>
<tr>
<td></td>
<td>( \log P = A - B/(C + T/K) )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \log P = A - B/(T/K) - C\log (T/K) )</td>
<td></td>
</tr>
</tbody>
</table>

\( A \), \( B \), \( C \)

- **Hertz & Rathmann 1912**
- **McDonald 1944**
- **Stull 1947**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>9733</td>
<td>17.8</td>
<td>4239</td>
<td>43.8</td>
<td>133.3</td>
</tr>
<tr>
<td>30.0</td>
<td>12266</td>
<td>19.85</td>
<td>7226</td>
<td>42.8</td>
<td>666.6</td>
</tr>
<tr>
<td>38.0</td>
<td>18532</td>
<td>20.99</td>
<td>7506</td>
<td>12.4</td>
<td>1333</td>
</tr>
<tr>
<td>44.15</td>
<td>23598</td>
<td>24.4</td>
<td>8813</td>
<td>1.0</td>
<td>2666</td>
</tr>
<tr>
<td>45.0</td>
<td>24398</td>
<td>25.5</td>
<td>9546</td>
<td>11.9</td>
<td>5333</td>
</tr>
<tr>
<td>51.0</td>
<td>31197</td>
<td>27.4</td>
<td>10319</td>
<td>20.0</td>
<td>7999</td>
</tr>
<tr>
<td>65.0</td>
<td>31329</td>
<td>30.2</td>
<td>11999</td>
<td>31.4</td>
<td>13332</td>
</tr>
<tr>
<td>77.0</td>
<td>74927</td>
<td>31.2</td>
<td>12426</td>
<td>48.0</td>
<td>26664</td>
</tr>
<tr>
<td>87.15</td>
<td>101325</td>
<td>34.39</td>
<td>14292</td>
<td>67.0</td>
<td>53329</td>
</tr>
<tr>
<td></td>
<td></td>
<td>38.49</td>
<td>17305</td>
<td>86.7</td>
<td>101325</td>
</tr>
<tr>
<td></td>
<td></td>
<td>39.29</td>
<td>18025</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>42.41</td>
<td>20545</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>44.51</td>
<td>22425</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>46.44</td>
<td>24318</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>51.05</td>
<td>29264</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>55.8</td>
<td>35210</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>60.5</td>
<td>41876</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>65.07</td>
<td>48889</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>71.44</td>
<td>61115</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>76.93</td>
<td>72988</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>80.38</td>
<td>81966</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>85.82</td>
<td>97018</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>86.47</td>
<td>98992</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( mp/°C; -73 \)
FIGURE 5.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.3
Reported Henry’s law constants of trichloroethylene at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{\text{AW}} &= A - B/(T/K) \quad (1) \\
\ln (1/K_{\text{AW}}) &= A - B/(T/K) \quad (2) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \quad (3) \\
\ln H &= A - B/(T/K) \quad (4) \\
K_{\text{AW}} &= A - B(T/K) + C(T/K)^2 \quad (5)
\end{align*}
\]

1. Leighton & Calo 1981 
2. Gossett 1987 
3. Ashworth et al. 1988 
4. Tancréde & Yanagisawa 90

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>240</td>
<td>1.0</td>
<td>254.4</td>
<td>15</td>
<td>675.8</td>
<td>25</td>
<td>768</td>
</tr>
<tr>
<td>1.2</td>
<td>231.2</td>
<td>1.75</td>
<td>324.2</td>
<td>20</td>
<td>853.2</td>
<td>27.4</td>
<td>999.5</td>
</tr>
<tr>
<td>2.5</td>
<td>307.1</td>
<td>34.6</td>
<td>1510</td>
<td>25</td>
<td>1034</td>
<td>28.9</td>
<td>828.7</td>
</tr>
<tr>
<td>7.0</td>
<td>366.4</td>
<td></td>
<td></td>
<td>30</td>
<td>1297</td>
<td>28.9</td>
<td>828.7</td>
</tr>
<tr>
<td>10.0</td>
<td>424.4</td>
<td>eq. 4</td>
<td>11.37</td>
<td></td>
<td></td>
<td>29.7</td>
<td>881.2</td>
</tr>
<tr>
<td>12.0</td>
<td>464.7</td>
<td>A</td>
<td>7.845</td>
<td></td>
<td></td>
<td>29.9</td>
<td>1159</td>
</tr>
<tr>
<td>12.0</td>
<td>484.8</td>
<td>B</td>
<td>4780</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12.9</td>
<td>523.4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.0</td>
<td>565.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18.0</td>
<td>683.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18.0</td>
<td>692.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18.0</td>
<td>683.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.0</td>
<td>717.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.2</td>
<td>761.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### TABLE 5.1.3.30.3 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>equilibrium cell-GC</td>
<td>EPICS-GC</td>
<td>EPICS-GC</td>
<td>EPICS-GC</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>19.5</td>
<td>723.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>24.3</td>
<td>979.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25.2</td>
<td>984.7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26.0</td>
<td>995.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26.0</td>
<td>1005</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26.1</td>
<td>1028</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 3</td>
<td>k_H/atm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>22.68</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>4735</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>activity coefficient</td>
<td>activity coefficient</td>
<td>headspace-GC</td>
<td>EPICS-GC</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>20</td>
<td>709</td>
<td>20</td>
<td>756</td>
<td>25</td>
</tr>
<tr>
<td>30</td>
<td>1155</td>
<td>30</td>
<td>1152</td>
<td>30</td>
</tr>
<tr>
<td>40</td>
<td>1753</td>
<td>40</td>
<td>1753</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>45</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>50</td>
</tr>
<tr>
<td>eq. 3</td>
<td>k_H/atm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>22.68</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>4735</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>static headspace-GC</td>
<td>calculated-P/C(measured)</td>
<td>SPME-GC</td>
<td>EPICS-SPME method</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m^3/mol)</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>15</td>
<td>575</td>
<td>21</td>
<td>703.4</td>
<td>15</td>
</tr>
<tr>
<td>20</td>
<td>709</td>
<td>50</td>
<td>2552</td>
<td>25</td>
</tr>
<tr>
<td>25</td>
<td>885</td>
<td>75</td>
<td>4934</td>
<td>30</td>
</tr>
<tr>
<td>30</td>
<td>1167</td>
<td>99</td>
<td>6854</td>
<td>40</td>
</tr>
<tr>
<td>35</td>
<td>1309</td>
<td>117</td>
<td>6127</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>1650</td>
<td></td>
<td></td>
<td>eq 1</td>
</tr>
<tr>
<td>45</td>
<td>2005</td>
<td></td>
<td></td>
<td>K_\text{aw}</td>
</tr>
<tr>
<td>eq. 3</td>
<td>k_H/atm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>8.62</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1736</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

eq. 1

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>K_\text{aw}</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>6.664</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td>2141</td>
<td></td>
</tr>
</tbody>
</table>

eq. 3

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>K_\text{aw}</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>11.121</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td>3648</td>
<td></td>
</tr>
</tbody>
</table>

eq. 1

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>K_\text{aw}</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>12.13</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td>3908.2</td>
<td></td>
</tr>
</tbody>
</table>
**FIGURE 5.1.1.30.3** Logarithm of Henry’s law constant versus reciprocal temperature for trichloroethylene.

**TABLE 5.1.1.30.4**

Reported octanol-water partition coefficients of trichloroethylene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K\text{ow}</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.2</td>
<td>2.18</td>
</tr>
<tr>
<td>6.0</td>
<td>2.18</td>
</tr>
<tr>
<td>10.0</td>
<td>2.28</td>
</tr>
<tr>
<td>14.1</td>
<td>2.24</td>
</tr>
<tr>
<td>18.7</td>
<td>2.29</td>
</tr>
<tr>
<td>24.8</td>
<td>2.20</td>
</tr>
</tbody>
</table>

change in enthalpy:

\[ \Delta H_{\text{ow}} / (\text{kJ mol}^{-1}) = 3.4 \]

(-8.4 to 15.2)

enthalpy of transfer

\[ \Delta H_{\text{oct}} / (\text{kJ mol}^{-1}) = 2.7 \]

(-9.0 to 14.5)
FIGURE 5.1.30.4 Logarithm of $K_{OW}$ versus reciprocal temperature for trichloroethylene.
5.1.1.31  Tetrachloroethylene

\[
\begin{array}{c}
\text{Cl} \\
\text{C} \\
\text{Cl} \\
\text{Cl} \\
\text{Cl}
\end{array}
\]

Common Name: Tetrachloroethylene  
Synonym: ethylene tetrachloride, perchloroethene, perchloroethylene, tetrachloroethene, 1,1,2,2-tetrachloroethylene  
Chemical Name: tetrachloroethylene  
CAS Registry No: 127-18-4  
Molecular Formula: \( \text{C}_2\text{Cl}_4, \text{CCl}_2=\text{CCl}_2 \)  
Molecular Weight: 165.833  
Melting Point (°C):  
\(-22.3\) (Lide 2003)  
Boiling Point (°C):  
121.3 (Lide 2003)  
Density (g/cm\(^3\) at 20°C):  
\( 1.62272, 1.61446 \) (20°C, 25°C, Dreisbach 1959)  
\( 1.6227 \) (Horvath 1982; Weast 1982-83)  
\( 1.62283, 1.61431 \) (20°C, 25°C, Riddick et al. 1986)  
Molar Volume (cm\(^3\)/mol):  
102.0 (20°C, calculated-density)  
128.0 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
39.61, 34.72 (25°C, bp, Riddick et al. 1986)  
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):  
10.56 (Riddick et al. 1986)  
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):  
150 (selected from literature or measured in DuPont laboratories, data also presented in graph, temp range 0-80°C, McGovern 1943)  
150 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)  
130, 120, 140 (1.5, 20, 25°C, selected from literature, Dilling 1977)  
200 (20°C, shake flask-GC, Chiou et al. 1977)  
400 (shake flask-GC, Freed et al. 1979)  
136 (37°C, shake flask-GC, Sato & Nakijima 1979)  
486 (shake flask-LSC, Banerjee et al. 1980)  
200 (shake flask-iteration/turbidity, Coca & Diaz 1980, Coca et al. 1980)  
478 (shake flask-LSC, Veith et al. 1980)  
150* (summary of literature data, temp range 0-80°C, Horvath 1982)  
242 (23–24°C, shake flask-GC, Broholm et al. 1992)  
286* (19.5°C, shake flask-GC/TC, measured range 0–91.8°C, Stephenson 1992)  
256 (activity coeff. by inert gas stripping-GC, Li et al. 1993)  
258.8 (20°C, limiting activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)  
206* (tentative value, temp range 0–70°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)  
\( S/(\text{wt}) = 0.26479 - 1.5487 \times 10^{-3}(T/K) + 2.4477 \times 10^{-6}(T/K)^2 \), temp range 273–343 K (equation derived from reported solubility data, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)  
192.3* (22°C, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range 22–161°C, Knauss et al. 2000)  
215 (deionized water, batch equilibrium, Ladaa et al. 2001)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666 (extrapolated, data presented in graph, McGovern 1943)

2397* (Antoine eq. regression, temp range –20.6 to 120.8°C, Stull 1947)

2462 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)

log (P/mmHg) = 7.02003 – 1415.5/(221.0 + t°C); temp range 34–187°C (Antoine eq. for liquid state, Dreisbach 1959)

2453* (vapor-liquid equilibrium VLE data, measured range 27.887–108°C, Polák et al. 1970)

log (P/mmHg) = 7.05854 – 1438.947/(233.368 + t°C); temp range 27.887–108°C (ebulliometry, Polák et al. 1970)


2394 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = –0.2185 × 9240.5/(T/K) + 8.026207; temp range –20.6 to 120.8°C (Antoine eq., Weast 1972–73)

2388 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 6.97183 – 1386.9/(217.526 + t°C); temp range 37–119°C (Antoine eq. from reported expptl. data, Boublik et al. 1973)

1866 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)

640, 1893, 2480 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)

2417, 2456 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.10343 – 1387.956/(217.64 + t°C), temp range: 37–120°C (Antoine eq. from reported expptl. data, Boublik et al. 1984)

2479, 4319 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

log (P/mmHg) = 30.4038 – 1.5265 × 10^3/(T/K) – 8.783·log (T/K) – 2.6364 × 10^-9·(T/K)^2; temp range 142–306 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2718 (exptl.-1/KAW = Cw/C_A, Hine & Mookerjee 1975)

248, 581 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)

1621 (20°C, batch stripping-GC, Mackay et al. 1979)

2006 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

log (H/atm) = 10.38 – 2159.0/(T/K) (least-square regression of data from lit., Kavanaugh & Trussell 1980)


ln (kH/atm) = 16.05 – 3539/(T/K); temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1528 (20°C, gas stripping-GC, Munz & Roberts 1982)

1316 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)

1317; 1175 (20°C, EPICS-GC; gas stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)

ln [H/(atm m³/mol)] = 13.12 – 5119/(T/K); temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)

ln [H/(atm m³/mol)] = 11.32 – 4622/(T/K); temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)

2908 (adsorption isotherm, Urano & Murata 1985)

1445 (20°C, multiple equilibration, Munz & Roberts 1986)

1852* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)

ln [H/(atm m³/mol)] = 12.45 – 4918/(T/K); temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)

1445 (20°C, EPICS-GC, Munz & Roberts 1987)

log KAW = 5.92 – 1802/(T/K); temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

© 2006 by Taylor & Francis Group, LLC
1106 Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals

\[ \ln \left[ \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right] = 10.65 - \frac{4368}{T/\text{K}}; \text{temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)} \]

\[ \log K_{\text{AW}} = 7.481 - \frac{2279}{T/\text{K}}; \text{temp range 25–47.2°C (EPICS-GC, Tancréde & Yanagisawa 1990)} \]

\[ \ln \left( \frac{1}{K_{\text{AW}}} \right) = -5.13 + 1736/(T/\text{K}); \text{temp range 2–25°C (equilibrium headspace-GC measurements, Kolb et al. 1992)} \]

\[ \gamma_\infty \text{ from gas stripping-GC, Li et al. 1993} \]

\[ \ln K_{\text{AW}} = -4528/(T/\text{K}) + 0.01080 \cdot Z + 14.655; \text{with } Z \text{ salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)} \]

\[ \log (kH/\text{atm}) = 9.06 – 1822/(T/\text{K}), \text{temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)} \]

\[ \log (kH/\text{atm}) = 9.09 – 1795/(T/\text{K}); \text{sea water 36‰ NaCl, temp range 15–45°C (headspace-GC measurements, Peng & Wan 1998)} \]

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\) at 25°C. Additional data at other temperatures designated * are compiled at the end of this section:

2.60 (shake flask-GC, Chiu et al. 1977)
2.60 (shake flask, Hansch & Leo 1979)
2.53 (shake flask-LSC, Banerjee et al. 1980)
2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
3.78 (HPLC-RT correlation, McDuffie 1981)
3.30, 2.72–3.57 (shake flask method: mean, range of mean values, OECD 1981)
3.40 (shake flask, Hansch & Leo 1985, 1987)
3.40 (correction of Ball & Roberts 1991 selection, Ball & Roberts 1992)
3.40 (recommended, Sangster 1993)
3.40 (recommended, Hansch et al. 1995)
2.27* (24.8°C, EPICS-GC, measured range 2.2–24.8°C Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\) at 25°C:

3.48 (head-space GC/FID, Abrahma et al. 2001)

Bioconcentration Factor, log BCF:

1.59 (trout, Neely et al. 1974)
1.598 (trout muscle, calculated-ratio of rate const. \(k_1/k_2\), Neely et al. 1974)
1.45–1.88 (calculated-\(K_{\text{OW}}\), Veith et al. 1979; Veith et al. 1980)
–1.70 (male Albino rats, Geyer et al. 1980)
1.69 (bluegill sunfish, Barrows et al. 1980)
1.49 (calculated-S, Kenaga 1980)
1.69 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
2.35 (calculated-$K_{ow}$, Lyman et al. 1982)
2.40 (microorganisms-water, Mabey et al. 1982)
2.06 (rainbow trout, Veith & Kosian 1982)
1.70 (calculated-MCI $\chi$, Koch 1983)
1.70, 2.30 (quoted, calculated, Sabljic 1987)
1.60 (calculated-solvatochromic parameters, Hawker 1990)
2.40 (calculated-$K_{ow}$, McCarty et al. 1992)
1.79 (rainbow trout, Saito et al. 1992)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
2.38 (calculated, Kenaga & Goring 1980, Kenaga 1980)
2.32 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
2.14; 2.54, 2.89; 2.35, 2.57 (calculated-$K_{ow}$; calculated-S and mp; calculated-S, Karickhoff 1981)
2.23 (average of 3 sediments and 5 soils, batch equilibrium, Schwarzenbach & Westall 1981)
2.04 (Schwarzenbach & Westall 1981)
3.23 (calculated-$K_{ow}$, Lyman et al. 1982)
2.38 (peaty soil, calculated-$K_{OM}$, Friesel et al. 1984)
2.56 (sediment-water, calculated-$K_{ow}$, Mabey et al. 1982)
2.56 (soil, Chiou et al. 1988)
2.00 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.76, 2.53 (organic cations treated Marlette soil A horizon; HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.75 (untreated Marlette soil Bt horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
2.87, 2.78 (organic cations treated Marlette soil B$_h$ horizon; HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.64 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
3.29 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
4.03 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
2.39, 2.57 (20°C, calculated-$K_{ow}$, Grathwohl 1990)
2.14 (calculated-molecular conductivity index, Olsen & Davis 1990)
2.45 (2.57% organic carbon in surface soil, Pignatello 1990, 1991)
1.81–2.95 (calculated-$K_{OM}$, Ball & Roberts 1991)
3.60 (Borden organic phase with no mineral sorption, Ball & Roberts 1991)
2.90 (Borden organic phase with no mineral sorption but with Curtis et al. 1986 correlation, Ball & Roberts 1992)
2.62, 2.79, 2.74, 2.80, 2.85, 2.78, 2.83 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
0.393–1.943 (19 soils from U.S. and China with polar organic carbon POC ranging form 2.89–59.9% and organic carbon OC ranging from 1.08–50.8%, batch sorption equilibrium, Kile et al. 1999)
1.13–2.11 (9 freshwater sediments from U.S. and China with polar organic carbon POC ranging form 5.36–52.5% and organic carbon OC ranging from 0.58–5.62%, batch sorption equilibrium, Kile et al. 1999)
2.32, 2.45, 2.22 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, 0.1 $\leq$ OC $< 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, log $K_{OM}$:
1.70 (untreated A horizon Marlette soil, Lee et al. 1989)
2.56, 2.30 (A horizon Marlette soil treated with HDTMA, DDTMA, Lee et al. 1989)
1.64 (untreated B horizon Marlette soil, Lee et al. 1989)
2.75, 2.64 (treated B, horizon Marlette soil with HDTMA, DDTMA, Lee et al. 1989)
2.32, 1.90 (quoted, calculated-molecular conductivity index, Olsen & Davis 1990)
3.20, 2.40 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
Environmental Fate Rate Constant, $k$, and Half-Lives, $t_{1/2}$:

Volatileization: evaporation $t_{1/2}({\text{exptl}}) = (27 \pm 3) \text{ min}$ for 1 mg/L in water when stirred at 200 rpm at approximately 25°C in an open container of 65 mm deep and $t_{1/2}({\text{calc}}) = 0.56 \text{ min}$ (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation $t_{1/2}({\text{exptl}}) = 20–27.1 \text{ min}$, $t_{1/2}({\text{calc}}) = 0.20, 26.5 \text{ min}$ at 20–25°C, and $t_{1/2}({\text{exptl}}) = 37.5 \text{ min}$, $t_{1/2}({\text{calc}}) = 27 \text{ min}$ at .15°C from water (Dilling 1977)

ratio of evaporation rate constant to that of oxygen reaeration: a measured value of 0.44 to that of 0.40 as predicted (Smith et al. 1980);

$\tau_{t} = 5–12 \text{ d}$ from pond, $t_{1/2} = 3 \text{ h-7 d}$ from river, $t_{1/2} = 3.6–14 \text{ d}$ from lake were estimated using representative reaeration rates (Lyman et al. 1982; quoted, Howard 1990);

estimated $t_{1/2} = 4.2 \text{ h}$ from water (Thomas 1982);

rate constants: $k = 0.028 \text{ d}^{-1}, t_{1/2} = 25 \text{ d}$ in spring at 8–16°C, $k = 0.051 \text{ d}^{-1}, t_{1/2} = 14 \text{ d}$ in summer at 20–22°C, $k = 0.056 \text{ d}^{-1}, t_{1/2} = 12 \text{ d}$ in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.057 \text{ d}^{-1}, t_{1/2} = 12.0 \text{ d}$ without HgCl$_2$ as poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: photocatalyzed mineralization by the presence of TiO$_2$ with the rate of 6.8 ppm/min per gram of catalyst (Ollis 1985); rate constant of $3.09 \times 10^{-3} \text{ h}^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O3} < 2 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Mathias et al. 1974; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime about 10 d (Yung et al. 1975; quoted, Callahan et al. 1979)

$k_{OH} = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow system-LMR, Howard 1976)

$k_{OH}^* = (1.69 \pm 0.07) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–420 K with calculated lifetime of 0.4–0.6 yr in troposphere (discharge flow system-RF, Chang & Kaufman 1977)

$k_{OH} = (0.13 \pm 0.04) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1978)

$k_{OH} = 1.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979, 1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)

$k_{OH} = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 68 d, loss of 1.5% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 1.0 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{O3} = 1.0 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (estimated, Lyman 1982)

$k << 100 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen 25°C (Mabey et al. 1982)

completely degraded in an hour (Dimitriades et al. 1983; quoted, Howard 1990)

$k < 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{O3} < 2 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH}^* = 1.67 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{OH}(\text{calc}) = 4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 1.0 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{NO3} < 4.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{NO3} < 4.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau > 240$ d, $k_{OH} = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with lifetime $\tau = 140$ d, and $k_{O3} < 2 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime $\tau > 2 \times 10^9$ yr at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.66 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{NO3} < 5.20 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to ethene at 298 ± 2 K (Atkinson 1991)

Hydrolysis: $k = 0.079 \text{ month}^{-1}$ at 25°C with $t_{1/2} = 8.8 \text{ months}$ (Dilling et al. 1975; quoted, Callahan et al. 1979); abiotic hydrolysis or dehydrohalogenation $t_{1/2} = 8.8 \text{ months}$ (Olsen & Davis 1990)

Biodegradation: aqueous aerobic $t_{1/2} = 4320–8640 \text{ h}$, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater grab sample test data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2352–39672 \text{ h}$, based on anaerobic screening test data (Bouwer et al. 1981; quoted, Howard et al. 1991); first-order $k = 1.1 \text{ yr}^{-1}$ with $t_{1/2} = 230 \text{ d}$ (Roberts et al. 1982; quoted, Olsen & Davis 1990)
Halogenated Aliphatic Hydrocarbons

\( t_{1/2} = 34 \text{ d} \) (Wood et al. 1985; quoted, Olsen & Davis 1990).
\( t_{1/2}\text{(aerobic)} = 180 \text{ d}, t_{1/2}\text{(anaerobic)} = 98 \text{ d} \) in natural waters (Capel & Larson 1995).

**Biotransformation:** estimated rate constant for bacteria \( k = 1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1} \) (Mabey et al. 1982).

**Bioconcentration, Uptake (k}_1 and Elimination (k}_2 Rate Constants or Half-Lives:**
- \( k_1 = 3.323 \text{ h}^{-1}; k_2 = 0.0823 \text{ h}^{-1} \) (trout muscle, Neely et al. 1974)
- \( k_1 = 11.4 \text{ h}^{-1} \) (flagfish, calculated-BCF \( \times k}_1, McCarty et al. 1992)
- \( k_2 = 0.0454 \text{ h}^{-1} \) (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)
- \( k_1 = 3.30 \text{ h}^{-1}; k_2 = 0.0833 \text{ h}^{-1} \) (trout, Hawker & Connell 1985)

**Half-Lives in the Environment:**

- **Air:**
  - tropospheric \( t_{1/2} = 12 \text{ wk} \), when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)
  - disappearance \( t_{1/2} > 10 \text{ d} \) for the reaction with OH radical (Darnall et al. 1976);
  - lifetime \( \sim 10 \text{ d} \), based on reaction with OH radical (Yung et al. 1975; quoted, Callahan et al. 1979);
  - photodecomposition \( t_{1/2} = 14.2 \text{ h} \) with NO and \( t_{1/2} = 8.3 \text{ h} \) with NO\(_2\) under simulated atmospheric conditions (Dilling et al. 1976);
  - estimated N. troposphere residence time of 150 d by one compartment nonsteady state model (Singh et al. 1978);
  - lifetime of 1.0 yr in troposphere (Altshuller 1980);
  - residence time of 68 d, loss of 1.5% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
  - estimated troposphere residence time of 200–390 d (Lyman 1982);
  - \( t_{1/2} = 384–3843 \text{ h} \), based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);
  - atmospheric lifetimes: \( \tau > 240 \text{ d} \) for the reaction with NO\(_3\) for a 12-h nighttime average concentration of \( 2.4 \times 10^4 \text{ molecule/cm}^3 \), \( \tau = 140 \text{ d} \) for the reaction with OH radical for a 12-h average concentration of \( 1.0 \times 10^4 \text{ molecule/cm}^3 \), and \( \tau > 2000 \text{ yr} \) for the reaction with O\(_3\) for a 24-h average concentration of \( 7 \times 10^1 \text{ molecule/cm}^3 \) (Atkinson et al. 1987).

- **Surface water:** estimated \( t_{1/2} = 9.9–32 \text{ d} \) in surface waters at various locations in case of a first order reduction process; \( t_{1/2} = 3–30 \text{ d} \) in rivers, \( t_{1/2} = 30–300 \text{ d} \) in lakes and ground waters (Zoeteman et al. 1980).
- \( t_{1/2} = 25 \text{ d} \) in spring at 8–16°C, 14 d in summer at 20–22°C and 12 d in winter at 3–7°C when volatilization dominates, and \( t_{1/2} = 12.1 \text{ d} \) and 12.0 d for experiments with and without HgCl\(_2\) as poison respectively in September 9–15 in marine mesocosm (Wakeham et al. 1983).
- \( t_{1/2} = 4320–8640 \text{ h} \), based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater sample grab data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991);
- calculated \( t_{1/2} = 10 \text{ d} \) and 32 d concentration reduction between sampling points on the Rhine River and a lake in the Rhine basin, respectively (Zoeteman et al. 1980; quoted, Howard 1990).
- \( t_{1/2}\text{(aerobic)} = 180 \text{ d}, t_{1/2}\text{(anaerobic)} = 98 \text{ d} \) in natural waters (Capel & Larson 1995).

- **Ground water:** \( t_{1/2} = 8640–17280 \text{ h} \), based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

- **Sediment:**
  - Soil: \( t_{1/2} < 10 \text{ d} \) (Ryan et al. 1988);
  - \( t_{1/2} = 4320–8640 \text{ h} \), based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

- **Biota:**
  - \( t_{1/2} < 1 \text{ d} \) in tissues of bluegill sunfish (Barrows et al. 1980);
  - \( t_{1/2} = 14 \text{ h} \), clearance from fish in simulated ecosystem (Neely 1980);
  - \( t_{1/2} < 10 \text{ d} \), subject to plant uptake via volatilization (Ryan et al. 1988);
  - \( t_{1/2} = 0.4–0.5 \text{ d} \) to eliminate from lsmall fish (McCarty et al. 1992).
TABLE 5.1.1.31.1
Reported aqueous solubilities of tetrachloroethylene at various temperatures

\[
S/(\text{wt\%}) = 1.49696 \times 10^{-2} - 7.8009 \times 10^{-6}(t/°C) - 5.1403 \times 10^{-7}(t/°C)^2 + 3.6938 \times 10^{-8}(t/°C)^3 \quad (1)
\]

\[
S/(\text{wt\%}) = 0.26479 - 1.5487 \times 10^{-3}(T/K) + 2.4477 \times 10^{-6}(T/K)^2 \quad (2)
\]

Horvath 1982
Stephenson 1992
Horvath & Getzen 1999a
Knauss et al. 2000

summary of literature data
shake flask-GC
summary of literature data
batch equilibrium-GC

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>149.7</td>
<td>0</td>
<td>273</td>
<td>0</td>
<td>244</td>
<td>23</td>
<td>192.3</td>
</tr>
<tr>
<td>10</td>
<td>148.8</td>
<td>9.5</td>
<td>270</td>
<td>5</td>
<td>234</td>
<td>51</td>
<td>247.4</td>
</tr>
<tr>
<td>20</td>
<td>149</td>
<td>19.5</td>
<td>286</td>
<td>10</td>
<td>224</td>
<td>75</td>
<td>313.8</td>
</tr>
<tr>
<td>25</td>
<td>150.3</td>
<td>31.1</td>
<td>221</td>
<td>15</td>
<td>218</td>
<td>101</td>
<td>519</td>
</tr>
<tr>
<td>30</td>
<td>152.7</td>
<td>40.0</td>
<td>213</td>
<td>20</td>
<td>211</td>
<td>124</td>
<td>1006</td>
</tr>
<tr>
<td>35</td>
<td>162</td>
<td>50.1</td>
<td>273</td>
<td>25</td>
<td>206</td>
<td>150</td>
<td>1895</td>
</tr>
<tr>
<td>40</td>
<td>179.1</td>
<td>61.3</td>
<td>304</td>
<td>30</td>
<td>202</td>
<td>161</td>
<td>2513</td>
</tr>
<tr>
<td>50</td>
<td>196.3</td>
<td>71</td>
<td>377</td>
<td>35</td>
<td>200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>245.7</td>
<td>80.2</td>
<td>380</td>
<td>40</td>
<td>198</td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>299.7</td>
<td>91.8</td>
<td>523</td>
<td>45</td>
<td>198</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 1.0 MPa</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1 S/wt%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>202</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>205</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>210</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>216</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 2 S/wt%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>temp range 273–343 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.1.31.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for tetrachloroethylene.
TABLE 5.1.1.31.2
Reported vapor pressures of tetrachloroethylene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–20.6</td>
<td>133.3</td>
<td>27.887</td>
<td>2869</td>
<td>37.088</td>
<td>4524</td>
</tr>
<tr>
<td>2.40</td>
<td>666.6</td>
<td>35.758</td>
<td>4274</td>
<td>52.671</td>
<td>9306</td>
</tr>
<tr>
<td>13.8</td>
<td>1333</td>
<td>41.702</td>
<td>5689</td>
<td>58.697</td>
<td>12046</td>
</tr>
<tr>
<td>26.3</td>
<td>2666</td>
<td>46.502</td>
<td>7101</td>
<td>63.270</td>
<td>14549</td>
</tr>
<tr>
<td>40.1</td>
<td>5333</td>
<td>57.065</td>
<td>11276</td>
<td>68.545</td>
<td>17921</td>
</tr>
<tr>
<td>49.2</td>
<td>7999</td>
<td>61.254</td>
<td>15412</td>
<td>73.064</td>
<td>21314</td>
</tr>
<tr>
<td>61.3</td>
<td>13332</td>
<td>68.065</td>
<td>17620</td>
<td>78.165</td>
<td>25780</td>
</tr>
<tr>
<td>79.8</td>
<td>26664</td>
<td>74.529</td>
<td>22541</td>
<td>82.292</td>
<td>29923</td>
</tr>
<tr>
<td>100.0</td>
<td>53329</td>
<td>81.957</td>
<td>29555</td>
<td>87.183</td>
<td>35493</td>
</tr>
<tr>
<td>120.8</td>
<td>101325</td>
<td>88.055</td>
<td>36557</td>
<td>91.791</td>
<td>41470</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–19.0</td>
<td>94.568</td>
<td>45465</td>
<td>97.291</td>
<td>49704</td>
</tr>
<tr>
<td></td>
<td></td>
<td>104.269</td>
<td>61875</td>
<td>103.930</td>
<td>61295</td>
</tr>
<tr>
<td></td>
<td></td>
<td>107.692</td>
<td>68694</td>
<td>111.548</td>
<td>77125</td>
</tr>
<tr>
<td></td>
<td></td>
<td>119.650</td>
<td>97337</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stull 1947

<table>
<thead>
<tr>
<th>summary of literature data</th>
</tr>
</thead>
<tbody>
<tr>
<td>log P = A – B/(T/K) (1)</td>
</tr>
<tr>
<td>log P = A – B/(C + t/°C) (2)</td>
</tr>
<tr>
<td>log P = A – B/(C + T/K) (3)</td>
</tr>
<tr>
<td>log P = A – B/(T/K) – C·log (T/K) (4)</td>
</tr>
</tbody>
</table>

Polak et al. 1970

<table>
<thead>
<tr>
<th>vapor-liquid equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>ln P = A – B/(T/K) (1a)</td>
</tr>
<tr>
<td>ln P = A – B/(C + t/°C) (2a)</td>
</tr>
</tbody>
</table>

Boublik & Aim 1972

<table>
<thead>
<tr>
<th>in Boublik et al. 1984</th>
</tr>
</thead>
<tbody>
<tr>
<td>eq. 2 P/kPa</td>
</tr>
<tr>
<td>A 6.10343</td>
</tr>
<tr>
<td>B 1387.956</td>
</tr>
<tr>
<td>C 217.640</td>
</tr>
<tr>
<td>bp 121.074</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
**FIGURE 5.1.1.31.2** Logarithm of vapor pressure versus reciprocal temperature for tetrachloroethylene.

**TABLE 5.1.1.31.3**
Reported Henry's law constants of tetrachloroethylene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>equilibrium cell-GC</td>
<td>EPICS-GC</td>
<td>EPICS-GC</td>
<td>equilibrium headspace-GC</td>
</tr>
<tr>
<td></td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>1.0</td>
<td>377.4</td>
<td>9.6</td>
<td>25</td>
<td>1363</td>
</tr>
<tr>
<td>1.0</td>
<td>413.5</td>
<td>17.5</td>
<td>26.5</td>
<td>1694</td>
</tr>
<tr>
<td>1.2</td>
<td>430.6</td>
<td>24.8</td>
<td>27.4</td>
<td>2224</td>
</tr>
<tr>
<td>2.5</td>
<td>474.9</td>
<td>34.6</td>
<td>28.9</td>
<td>2160</td>
</tr>
<tr>
<td>7.0</td>
<td>572.9</td>
<td></td>
<td>28.9</td>
<td>2034</td>
</tr>
<tr>
<td>10.0</td>
<td>675.2</td>
<td></td>
<td>29.7</td>
<td>2770</td>
</tr>
<tr>
<td>12.0</td>
<td>731.4</td>
<td>eq. 4</td>
<td>29.9</td>
<td>2998</td>
</tr>
<tr>
<td>12.0</td>
<td>797.6</td>
<td>A</td>
<td>33.3</td>
<td>3057</td>
</tr>
<tr>
<td>12.9</td>
<td>826.0</td>
<td>B</td>
<td>35.6</td>
<td>2413</td>
</tr>
<tr>
<td>14.0</td>
<td>914.7</td>
<td></td>
<td>38.3</td>
<td>2745</td>
</tr>
<tr>
<td>18.0</td>
<td>1122</td>
<td></td>
<td>40</td>
<td>4895</td>
</tr>
<tr>
<td>18.0</td>
<td>1144</td>
<td></td>
<td>44.7</td>
<td>5549</td>
</tr>
<tr>
<td>18.0</td>
<td>1145</td>
<td></td>
<td>45</td>
<td>6004</td>
</tr>
<tr>
<td>19.0</td>
<td>1176</td>
<td></td>
<td>47.2</td>
<td>5886</td>
</tr>
<tr>
<td>19.2</td>
<td>1156</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.5</td>
<td>1182</td>
<td>10</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

References:
- Leighton & Calo 1981
- Gossett 1987
- Tancréde & Yanagisawa 1990
- Kolb et al. 1992

Equations:

1. \( \ln K_{AW} = A - B/ (T/K) \) (1)
2. \( \ln (1/K_{AW}) = A - B/ (T/K) \) (2)
3. \( \ln [H/(Pa \cdot m^3/mol)] = A - B/ (T/K) \) (3)
4. \( \ln [H/(atm \cdot m^3/mol)] = A - B/ (T/K) \) (4)
5. \( K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \) (5)
### TABLE 5.1.1.31.3 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>equilibrium cell-GC</td>
<td>EPICS-GC</td>
<td>EPICS-GC</td>
<td>equilibrium headspace-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>24.3</td>
<td>1583</td>
<td>15</td>
<td>1125</td>
</tr>
<tr>
<td>25.2</td>
<td>1623</td>
<td>20</td>
<td>1429</td>
</tr>
<tr>
<td>25.3</td>
<td>1651</td>
<td>25</td>
<td>1733</td>
</tr>
<tr>
<td>26.0</td>
<td>1636</td>
<td>30</td>
<td>2482</td>
</tr>
<tr>
<td>26.1</td>
<td>1712</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>headspace-GC</td>
<td>EPICS-GC</td>
<td>equilibrium headspace-GC</td>
<td>calculated-P/C</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>25</td>
<td>1723</td>
<td>2.0</td>
<td>359.2</td>
</tr>
<tr>
<td>30</td>
<td>2340</td>
<td>6.0</td>
<td>2492</td>
</tr>
<tr>
<td>40</td>
<td>3070</td>
<td>10.0</td>
<td>602.7</td>
</tr>
<tr>
<td>45</td>
<td>2847</td>
<td>18.2</td>
<td>995.6</td>
</tr>
<tr>
<td>45.0</td>
<td>2713</td>
<td>45</td>
<td>4108</td>
</tr>
<tr>
<td>40</td>
<td>1490</td>
<td>eq. 1</td>
<td>K_{AW}</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>14.655</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td>4528</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 3a</td>
<td>k'H/atm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 5.1.1.31.3** Logarithm of Henry’s law constant versus reciprocal temperature for tetrachloroethylene.
TABLE 5.1.1.31.4
Reported octanol-water partition coefficients of tetrachloroethylene at various temperatures

Dewulf et al. 1999

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.2</td>
<td>2.25</td>
</tr>
<tr>
<td>6.0</td>
<td>2.27</td>
</tr>
<tr>
<td>10.0</td>
<td>2.38</td>
</tr>
<tr>
<td>14.1</td>
<td>2.32</td>
</tr>
<tr>
<td>18.7</td>
<td>2.36</td>
</tr>
<tr>
<td>24.8</td>
<td>2.27</td>
</tr>
</tbody>
</table>

change in enthalpy:
\[ \Delta H_{OW}/(kJ \text{ mol}^{-1}) = 2.6 \]
\[ (-11.1 \text{ to } 16.3) \]

enthalpy of transfer
\[ \Delta H_{oct}/(kJ \text{ mol}^{-1}) = 4.7 \]
\[ (-9.0 \text{ to } 18.4) \]

FIGURE 5.1.1.31.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloroethylene.
5.1.1.32 1,3-Dichloropropene

Common Name: 1,3-Dichloropropene
Synonym: 1,3-dichloropropylene, 1,3-dichloro-1-propene, Telone II
Chemical Name: 1,3-dichloropropene
CAS Registry No: 542-75-6
Molecular Formula: C₃H₄Cl₂, CH₂ClCH=CHCl
Molecular Weight: 110.970
Melting Point (°C):
Boiling Point (°C):
  112.0 (trans-stereoisomer I, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)
  104.3 (cis-stereoisomer II, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
  1.224 (trans-stereoisomer I, Horvath 1982; McNally & Grob 1984)
  1.217 (cis-stereoisomer II, Horvath 1982; McNally & Grob 1984)
Molar Volume (cm³/mol):
  91.2 (trans-stereoisomer I, 20°C, calculated-density)
  90.7 (cis-stereoisomer II, 20°C, calculated from density)
  108.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  2800 (trans-stereoisomer I, Dilling 1977)
  2700 (cis-stereoisomer II, Dilling 1977)
  2723 (recommended, Horvath 1982)
  1071 (trans-stereoisomer I, headspace-GC, McNally & Grob 1983)
  1088 (cis-stereoisomer II, headspace-GC, McNally & Grob 1983)
  1020 (30°C, trans-stereoisomer I, headspace-GC, McNally & Grob 1984)
  911 (30°C, cis-stereoisomer II, headspace-GC, McNally & Grob 1984)
  1000 (20°C, Wauchope et al. 1992)
  2250 (Wauchope et al. 1992)
  4533, 4311, 4223 (20, 30, 40°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated):
  4533, 5733 (trans-, cis-stereoisomer, data from Dow Chemicals, Dilling 1977)
  435, 569 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
  3333 (20°C, selected, Mills et al. 1982)
  3334 (20°C, quoted, Warner et al. 1987)
  3866 (20°C, Wauchope et al. 1992)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
  232 (calculated-P/C, Dilling 1977)
  137 (calculated-P/C, Warner et al. 1987)
  122, 198, 302 (20, 30, 40°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
Octanol/Water Partition Coefficient, log K_{ow}:
  1.98 (selected, Mills et al. 1982)
  1.41 (quoted, Verhaar et al. 1992)
  1.84 (cis/trans, calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

1.505  
(soil, selected, Wauchope et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatileization: t_{1/2} = 31 min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975)

\[ t_{1/2}(\text{exptl}) = 29.6 \text{ min, } t_{1/2}(\text{calc}) = 2.4 \text{ min, } 23.8 \text{ min for cis-stereoisomer, and } t_{1/2}(\text{calc}) = 3.2 \text{ min, } 24.6 \text{ min for trans-stereoisomer from water} \] (Dilling 1977)

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO3 radical and k_{O3} with O3 or as indicated, *data at other temperatures see reference:

\[ k_{OH} = (7.74 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ cis-isomer}, k_{OH} = (1.31 \pm 0.05) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trans-isomer at } 22 \pm 2^\circ C, \text{ calculated } t_{1/2} = 12 \text{ h and 7 h for the cis- and trans-isomer, respectively (relative rate method, Tuazon et al. 1984)}

\[ k_{O3} = 1.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ cis-isomer}, k_{O3} = 6.7 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trans-isomer at room temp., calculated } t_{1/2} = 52 \text{ d and 12 d for cis- and trans-isomer, respectively (relative rate method, Tuazon et al. 1984)}

Hydrolysis: t_{1/2} = 133–271 h, based on measured rate constants for hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991); rate of hydrolysis is, however, independent of pH over the range of pH 5 to pH 10 (McCall 1987).

Biodegradation: aerobic t_{1/2} = 168–672 h, based on unacclimated aerobic biodegradation screening studies (Tabak et al. 1981; Krijgheld & Van der Gen 1986; quoted, Howard et al. 1991); anaerobic t_{1/2} = 672–2688 h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).
5.1.1.33  Chloroprene

Common Name: Chloroprene
Synonym: 2-chloro-1,3-butadiene
Chemical Name: 2-chloro-1,3-butadiene
CAS Registry No: 126-99-8
Molecular Formula: C₄H₅Cl, CH₂=CClCH=CH₂
Molecular Weight: 88.536

Melting Point (°C):

-130  (Kirk-Othmer 1985; Verschueren 1983; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

59.4  (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
69.145  (Boublik et al. 1984)

Density (g/cm³ at 20°C):

0.9583  (Weast 1982–83; Dean 1985)
0.9580  (Verschueren 1983)

Molar Volume (cm³/mol):

92.4  (20°C, calculated-density, Stephenson & Malanowski 1987)
102.3  (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_fus (kJ/mol):

Entropy of Fusion, ΔS_fus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

964000  (20°C, saturation concentration, Verschueren 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

26660, 36660  (20°C, 30°C, Verschueren 1983)
28740  (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.30955 – 793.85/(181.137 + t°C), temp range: 20–60°C (Antoine eq. from reported exptl. data
Boublik et al. 1984)
28780  (interpolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.16150 – 783.45/(197.7 + t°C); temp range 20–60°C (Antoine eq., Dean 1985, 1992)
29450  (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_t/kPa) = 6.652 – 1545.3/(T/K); temp range: 279–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_t/kPa) = 6.6519 – 1545.0/(T/K); temp range 243–263 K (Antoine eq.-II, Stephenson & Malanowski 1987)
23200  (quoted, Howard 1989)

log (P/mmHg) = 8.9353 – 1.9176 × 10³/(T/K) + 0.73836·log (T/K) – 8.4743 × 10⁻³·(T/K) + 6.0224 × 10⁻⁶·(T/K)²;
  temp range 143–525 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

3242  (estimated by bond contribution method, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW}:

2.03  (Howard 1989)

Bioconcentration Factor, log BCF:

1.342  (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

2.498  (soil, estimated-K_{OW}, Lyman et al. 1982)
1.699 (soil, molecular topology and QSAR, Sabljic 1984)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatileization: $t_{1/2} \approx 3$ h from a model river 1 m deep with a current velocity of 1 m/s and a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1989).

Photolysis:
Oxidation: photooxidation $t_{1/2} = 2.9–27.8$ h, based on estimated rate constants for the reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:
Biodegradation: aqueous aerobic $t_{1/2} = 672–4320$ h, based on aqueous aerobic screening test data for vinyl chloride (Helfgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688–17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24–2.4$ h from air for the reaction with OH radicals (Darnall et al. 1976);
- $t_{1/2} = 1.8$ h for the reaction with photochemically produced hydroxyl radicals and $t_{1/2} = 12$ h for the reaction with ozone in atmosphere (Cupitt 1980; quoted, Howard 1989);
- $t_{1/2} = 2.9–27.8$ h, based on estimated rate constants for reaction with hydroxyl radicals and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated $t_{1/2} = 6.7–53$ d in surface waters at various locations in case of a first order reduction process; and $t_{1/2} = 3–30$ d in rivers, $t_{1/2} = 30–300$ d in lakes and ground waters (Zoeteman et al. 1980)
- $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344–8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
5.1.1.34 Hexachlorobutadiene

Common Name: Hexachlorobutadiene
Synonym: HCBD, perchloro-1,3-butadiene
Chemical Name: 1,1,2,3,4,4-hexachloro-1,3-butadiene
CAS Registry No: 87-68-3
Molecular Formula: C₄Cl₆, Cl₂C=CClIClC=CCl₂
Molecular Weight: 260.761
Melting Point (°C): -21.0 (Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C): 215 (Horvath 1982; Lide 2003)
Density (g/cm³ at 20°C): 1.682 (Horvath 1982)
Molar Volume (cm³/mol):
155.2 (20°C, calculated-density, Stephenson & Malanowski 1987)
206.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.20 (Melnikov 1971)
2.00 (20°C, Pearson & McConnell 1975)
3.23 (shake flask-HPLC, Banerjee et al. 1980)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
20.0 (20°C, Pearson & McConnell 1975)
log (P/kPa) = 6.06503 – 1520.873/(163.685 + t°C); temp range 70–200°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.4781 – 1783.8/(–84.48 + T/K); temp range 343–484 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
2604 (calculated-P/C, Warner et al. 1987)
1044 (batch stripping, Warner et al. 1987)
Octanol/Water Partition Coefficient, log K_{OW}:
4.74 (HPLC-RT correlation, Konemann et al. 1979)
4.78 (shake flask-HPLC, Banerjee et al. 1980)
4.63 (calculated-fragment const., Könemann 1981)
4.90 (shake flask-GC, both phases, Chiu 1985)
4.78 (recommended, Sangster 1993)
4.78 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
4.70 (Thomann 1989)
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2965–28650$ h, based on an estimated rate constant for vapor phase reaction with OH radicals (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable groups, rate constant at pH 7 is zero (Kollig et al. 1987).

Biodegradation: aqueous aerobic $t_{1/2} = 672–4320$ h, based on monitoring data and acclimated aqueous screen test data (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688–17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} \sim 1.0$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

$\text{t}_{1/2} = 2865–28650$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 672–4320$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344–8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
5.1.1.35 Hexachlorocyclopentadiene

Common Name: Hexachlorocyclopentadiene
Synonym: 1,2,3,4,5,5-hexachlorocyclopentadiene, perchlorocyclopentadiene, HCCPD
Chemical Name: 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene
CAS Registry No: 77-47-4
Molecular Formula: C₅Cl₆
Molecular Weight: 272.772
Melting Point (°C):
-9  (Lide 2003)
Boiling Point (°C):
239  (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C): 1.702
Molar Volume (cm³/mol):
160.3  (20°C, calculated-density, Stephenson & Malanowski 1987)
210.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.805  (Shake flask-LSC Lu et al. 1974)
1.80  (Zepp et al. 1979)
0.805  (Callahan et al. 1979; Dobbs et al. 1980; Geyer et al. 1981; Warner et al. 1987; Isnard & Lambert 1988)
1.80  (28°C, vapor saturation or shake flask-GC, Wolfe et al. 1982)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
10.84  (Verschueren 1977; Warner et al. 1987)
10.67  (Wolfe et al. 1982)
11.90  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/µPa) = 7.4813 - 2804.32/(T/K); temp range 335–512 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = -9.7942 – 3.3161 × 10³/(T/K) + 10.171-log (T/K) – 2.1115 × 10⁻²·(T/K) + 9.2045 × 10⁻⁶·(T/K)²;
temp range 284–746 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol):
2736  (concentration ratio-GC, Wolfe et al. 1982)
1662  (batch stripping; Warner et al. 1987)
Octanol/Water Partition Coefficient, log K_{ow}:
5.04  (HPLC-RT correlation, McDuffie 1981)
5.04  (28°C, concentration ratio-GC, Wolfe et al. 1982)
5.26  (HPLC-RT correlation, Eadsforth 1986)
5.04  (recommended, Sangster 1993)
5.04  (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
2.53, 2.97, 3.21, 2.65 (algae, snail, mosquito, fish, Lu et al. 1975)
1.47  (fathead minnow, Veith et al. 1979)
3.04, 3.21  (Chlorella, calculated-solubility, Geyer et al. 1981)
Sorption Partition Coefficient, log $K_{OC}$:
4.08 (sediment organic carbon, calculated-$K_{OW}$, Wolfe et al. 1982)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

- Volatilization: appears to be important in flowing waters (Callahan et al. 1979).
  - Photolysis: near-surface photolysis is an important process with a rate constant $k = 4.9 \text{ d}^{-1}$ with $t_\frac{1}{2} = 11 \text{ min}$ (Callahan et al. 1979);
  - direct photolysis in natural waters in midday sunlight of Athens, Georgia at latitude 34°N and 83°W with $t_\frac{1}{2} < 10 \text{ min}$, and near-surface photolysis rate constant $k(\text{calc}) = 3.9 \text{ h}^{-1}$ on cloudless days averaged over both light and dark periods for a year (Wolfe et al. 1982);
  - photolysis $t_\frac{1}{2} = 1.0 \text{ min}$ to 10.7 min, based on photolysis studies in aqueous solutions (Butz et al. 1982; Wolfe et al. 1982; quoted, Howard et al. 1991).
- Oxidation: photooxidation $t_\frac{1}{2} = 1.0$ to 8.9 h, based on calculated rate constants for the vapor phase reactions with OH radicals and O$_3$ in air (Cupitt 1980; quoted, Howard et al. 1991).
- Hydrolysis: appears to be an important fate process with a rate constant $k = 5.6 \times 10^{-7} \text{ s}^{-1}$ at 25°C with $t_\frac{1}{2} = 14 \text{ d}$ (Callahan et al. 1979);
  - reaction rate constant was independent of pH range of about 3 to 10 under most environmental conditions and an extrapolated rate constant $l = 4 \times 10^{-3} \text{ s}^{-1}$ was found at 25°C with $t_\frac{1}{2} = 173 \text{ h}$ (Wolfe et al. 1982; quoted, Howard et al. 1991).
- Biodegradation: aqueous aerobic $t_\frac{1}{2} = 168$ to 672 h, based on aerobic aqueous screening test data (Tabak et al. 1981; Freitag et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_\frac{1}{2} = 672$ to 2688 h, based on aerobic aqueous biodegradation half-life (Howard et al. 1991).
- Biotransformation:
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

- Air: $t_\frac{1}{2} = 1.0$ to 8.9 h, based on estimated photooxidation half-life in air (Howard et al. 1991).
- Surface water: $t_\frac{1}{2} = 1.0 \text{ min}$ to 173 h, based on photolysis and hydrolysis half-lives (Howard et al. 1991); measured rate constant $k = (90 \pm 40) \text{ M}^{-1} \text{s}^{-1}$ for direct reaction with ozone in water at pH 2 and 25 ± 2°C, with $t_\frac{1}{2} = 6 \text{ min}$ at pH 7 (Yao & Haag 1991).
- Ground water: $t_\frac{1}{2} = 173$ to 1344 h, based on aerobic aqueous biodegradation and hydrolysis half-lives (Howard et al. 1991).
- Sediment: hydrolysis rate constant in the sediment was assumed to be the same as that of water and decay rate constant $k = 1.5$ to $5.4 \times 10^{-5} \text{ s}^{-1}$ for natural pond sediment-water system (Wolfe et al. 1982).
- Soil: $t_\frac{1}{2} = 168$ to 672 h, based on aerobic aqueous biodegradation half-life (Howard et al. 1991).
5.1.2  Bromoalkanes and Bromoalkenes

5.1.2.1  Bromomethane

\[
\begin{align*}
\text{H} & \quad \text{H} \quad \text{Br} \\
\text{H} &
\end{align*}
\]

Common Name: Methyl bromide  
Synonym: bromomethane, monobromomethane, Embafume, Terabol  
Chemical Name: bromomethane, methyl bromide  
CAS Registry No: 74-83-9  
Molecular Formula: CH₃Br  
Molecular Weight: 94.939  
Melting Point (°C):  
–93.68  (Lide 2003)  
Boiling Point (°C):  
3.5  (Lide 2003)  
Density (g/cm³ at 20°C):  
1.6755, 1.6617  (20°C, 25°C, Dreisbach 1961)  
Molar Volume (cm³/mol):  
56.7  (20°C, calculated-density)  
52.9  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):  
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):  
13410*  (vapor saturation-gravitational method, measured range 10–32°C, Haight 1951)  
14400  (Irmann 1965; Hine & Mookerjee 1975)  
13400  (Jolles 1966; Günther et al. 1968)  
12930  (Korenman et al. 1971)  
900  (20°C, Verschueren 1977, 1983)  
15223*  (summary of literature data, temp range 5–80°C, Horvath 1982)  
17500  (20°C, Windholz et al. 1983)  

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
256550  (interpolated-Antoine eq. regression, temp range –96.3 to 3.6°C, Stull 1947)  
217700  (calculated-Antoine eq., Dreisbach 1959, 1961)  
\[
\log (P/\text{mmHg}) = 6.95965 – 986.59/(238.32 + t/°C); \text{ temp range } –58 \text{ to } 53°C \quad (\text{Antoine eq. for liquid state,}\n\text{Dreisbach 1959, 1961})
\]
\[
\log (P/\text{mmHg}) = 6.95965 – 986.590/(238.32 + t/°C); \text{ pressure range of } 10 \text{ to } 1500 \text{ mmHg} \quad (\text{Antoine eq. from correlation of selected lit. data,} Li \text{ and Rossini 1961})
\]
183900  (calculated-Antoine eq., Weast 1972–73)  
\[
\log (P/\text{mmHg}) = [-0.2185 \times 5925.9/(T/K)] + 7.482362; \text{ temp range } –96.3 \text{ to } 190°C \quad (\text{Antoine eq., Weast 1972–73})
\]
218930  (calculated-Antoine eq., Kudchadker et al. 1979)  
\[
\log (P/\text{mmHg}) = 7.08823 – 1044.42/(244.684 + t/°C); \text{ temp range } –96.3 \text{ to } 190°C \quad (\text{Antoine eq., Kudchadker et al. 1979})
\]
187000  (20°C, Thomas 1982)  
216900, 219000  (calculated-Antoine eq., Boublik et al. 1984)  
\[
\log (P/\text{Pa}) = 6.20369 – 1041.723/(244.36 + t/°C); \text{ temp range } –69.9 \text{ to } 4.5°C \quad (\text{Antoine eq. from reported expctl. data, Boublik et al. 1984})
\]
log (P/kPa) = 6.2243 – 1049.898/(245.319 + t/°C); temp range –70 to 3.6°C (Antoine eq. from reported expn. data, Boublik et al. 1984)

log (P/kPa) = 6.21313 – 1044.42/(224.684 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

217680 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 29.3988 – 2.0406 × 103/(T/K) – 7.9966·log (T/K) + 4.1899 × 10–10·(T/K)2; temp range 179–467 K (vapor pressure eq., Yaws 1994)

218630 (selected and summary of literature data, temp range 179.48–318.15 K, Xiang 2002)

Henry’s Law Constant (Pa m3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

631*; 621 (exptl.-conc. ratio, measured range 5–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)

log {H/(mmHg·L/mol)} = 73.022 – 22.261·log (T/K) – 4254.8/(T/K); temp range 278.16–253.16 K (Glew & Moelwyn-Hughes 1953)

733* (29.43°C, concentration ratio, measured range 29.44–49.59°C, Swain & Thornton 1962)

652 (calculated as I/KAw, Cw/Ca, reported as expn., Hine & Mookerjee 1975)

533 (20°C, calculated-P/C, Mackay & Shiu 1981)

19958 (20°C, calculated-P/C, Mabey et al. 1982)

1317 (calculated-P/C, Thomas 1982)

20260 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

10690 (calculated-P/C, Mackay & Shiu 1990)

687.4 (computed value, Yaws et al. 1991)

204, 515 (0, 22°C, distilled water, headspace-GC, Elliott & Rowland 1993)

596* (gas-liquid equilibrator-GC, measured range 1.1–30.5°C, De Bruyn & Saltzman 1997)

490 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

log KAw = 3.468 – 1221/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kow:

1.19 (shake flask-GC, Leo et al. 1975)

1.19 (Hansch & Leo 1979; Hansch & Leo 1985)

1.19 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log Koa:

2.11 (calculated-infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.623 (microorganisms-water, calculated-Kow, Mabey et al. 1982)

0.672 (calculated-Kow, Lyman et al. 1982)

Sorption Partition Coefficient, log Koc:

2.236, 2.241, 2.215 (Naaldwijk loamy sand, Aalsmeer loam, Boskoop peaty clay, Howard 1989)

0.771 (sediment-water, calculated-Kow, Mabey et al. 1982)

2.10 (calculated-S, Lyman et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization: estimated experimental t½ = 27 min 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979); t½ ~ 30 min (Mills et al. 1982);

VOC = 3.0 h in a model river (estimated, Lyman et al. 1982; quoted, Howard 1989);

VOC ~ 0.2 and 0.5 d for the volatilization from 1 and 10 cm of soil, respectively (Jury et al. 1984; quoted, Howard 1989).

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$k_{OH}^* = (4.14 \pm 0.43) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 245–375 K with lifetime of 1.32 yr in the troposphere (flash photolysis-RF, Davis et al. 1976)

$k_{OH} = 3.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow system, Howard & Evenson 1976)

$k_{OH} = 4.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 289 d, loss of 0.4% in one day or 12 sunlit hour at 300 K (Singh et al. 1981)

$k_{OH} = 2.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (estimated, Lyman 1982)

$k_{OH}^* = 3.93 \times 10^{-14} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 0.1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{1/2} = 1633–16327 \text{ h}$ in air, based on measured rates for reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: first-order $k = 4.0 \times 10^{-7} \text{ s}^{-1}$ with a maximum $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979);

$k = 4.09 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978)

$\text{half-life} = 470–912 \text{ h}$, based on measured first-order hydrolysis rate constants (Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard 1989; Howard et al. 1991);

$k = 1.44 \times 10^{-3} \text{ h}^{-1}$ at pH 7 and 25°C (Callahan et al. 1979; quoted, Mabey et al. 1982)

$k = 3 \times 10^{-7} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 26.7 \text{ d}$ (Castro & Belser 1981; quoted, Howard 1989).

Biodegradation: aerobic $t_{1/2} (\text{aq.}) = 168–672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

anaerobic $t_{1/2} (\text{aq.}) = 672–2688 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Tabak et al. 1981; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24 \text{ h}$ from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

time of 3.8 yr in the troposphere (Altshuller 1980);

$\text{half-life} = 0.29 \text{ y}$ in the atmosphere for the reaction with $2 \times 10^5 \text{ OH radicals/cm}^3$ at 25°C (Dilling 1982; quoted, Howard 1989);

$\text{half-life} = 289 \text{ d}$ estimated as toxic chemical residence time with rate constant of $4 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals at 300 K (Singh et al. 1980,1981; quoted, Howard 1989);

$\text{half-life} = 1633–16327 \text{ h}$, based on measured rates for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$\text{half-life} = 168–672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 336–912 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic waste water inoculum and hydrolysis half-life (Tabak et al. 1981; Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168–672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:
TABLE 5.1.2.1.1
Reported aqueous solubilities of bromomethane at various temperatures

\[
S/(\text{wt\%}) = 1.4019 - 6.3562 \times 10^{-2}(t/\degree \text{C}) + 1.71977 \times 10^{-3}(t/\degree \text{C})^2
+ 2.5268 \times 10^{-7}(t/\degree \text{C})^4 - 9.3470 \times 10^{-10}(t/\degree \text{C})^5 \tag{1}
\]

Haight 1951

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>26790</td>
<td>5</td>
<td>35000</td>
</tr>
<tr>
<td>17</td>
<td>18300</td>
<td>10</td>
<td>27997</td>
</tr>
<tr>
<td>25</td>
<td>13410</td>
<td>20</td>
<td>18401</td>
</tr>
<tr>
<td>32</td>
<td>11490</td>
<td>25</td>
<td>15223</td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>30</td>
<td>12804</td>
</tr>
<tr>
<td>40</td>
<td>9517</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>7430</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>5919</td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>4757</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Horvath 1982

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>35000</td>
</tr>
<tr>
<td>10</td>
<td>27997</td>
</tr>
<tr>
<td>20</td>
<td>18401</td>
</tr>
<tr>
<td>25</td>
<td>15223</td>
</tr>
<tr>
<td>30</td>
<td>12804</td>
</tr>
<tr>
<td>40</td>
<td>9517</td>
</tr>
<tr>
<td>50</td>
<td>7430</td>
</tr>
<tr>
<td>60</td>
<td>5919</td>
</tr>
<tr>
<td>70</td>
<td>4757</td>
</tr>
</tbody>
</table>

eq. 1 S/wt%

FIGURE 5.1.2.1.1  Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromomethane.
TABLE 5.1.2.1.2
Reported Henry's law constants of bromomethane at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \\
\ln (1/K_{AW}) &= A - B/(T/K) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \\
\ln H &= A - B/(T/K) \\
K_{AW} &= A - B(T/K) + C(T/K)^2 \\
\log H &= A - B\log (T/K) - C/(T/K)
\end{align*}
\]

Glew & Moelwyn-Hughes 1953
Swain & Thornton 1962
De Bruyn & Saltzman 1997

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>pure water</th>
<th>seawater</th>
<th>35% NaCl</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.0</td>
<td>276</td>
<td>29.43</td>
<td>729</td>
<td>1.1</td>
<td>205.5</td>
<td>253.9</td>
<td>255.2</td>
</tr>
<tr>
<td>10.0</td>
<td>340</td>
<td>29.43</td>
<td>733</td>
<td>5.0</td>
<td>261.8</td>
<td>321.7</td>
<td>320.6</td>
</tr>
<tr>
<td>14.98</td>
<td>427</td>
<td>29.44</td>
<td>744</td>
<td>10.0</td>
<td>334.4</td>
<td>424.0</td>
<td>417.0</td>
</tr>
<tr>
<td>20.0</td>
<td>532</td>
<td>40.35</td>
<td>980</td>
<td>13.4</td>
<td>380.9</td>
<td>471.3</td>
<td>460.6</td>
</tr>
<tr>
<td>24.97</td>
<td>631</td>
<td>40.35</td>
<td>992</td>
<td>18.0</td>
<td>440.5</td>
<td>536.1</td>
<td>-</td>
</tr>
<tr>
<td>30.0</td>
<td>744</td>
<td>40.35</td>
<td>1005</td>
<td>19.4</td>
<td>458.5</td>
<td>-</td>
<td>539.0</td>
</tr>
<tr>
<td>40.05</td>
<td>1005</td>
<td>49.59</td>
<td>1253</td>
<td>21.2</td>
<td>494.3</td>
<td>-</td>
<td>566.1</td>
</tr>
<tr>
<td>50.04</td>
<td>1301</td>
<td></td>
<td></td>
<td>25.0</td>
<td>596.0</td>
<td>708.6</td>
<td>666.1</td>
</tr>
<tr>
<td>60.03</td>
<td>1653</td>
<td></td>
<td></td>
<td>30.5</td>
<td>666.6</td>
<td>810.6</td>
<td>761.8</td>
</tr>
<tr>
<td>70.0</td>
<td>1987</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.0</td>
<td>2400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25.0</td>
<td>622</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

eq 6 \( P/(\text{mmHg} \cdot \text{L/mol}) \)

A \( 73.022 \)
B \( 22.261 \)
C \( 4254.8 \)

FIGURE 5.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for bromomethane.
5.1.2.2 Dibromomethane

\[
\begin{align*}
\text{H} & \\
\text{Br} & \text{Br} \\
\text{H} & 
\end{align*}
\]

Common Name: Dibromomethane
Synonym: methylene bromide
Chemical Name: dibromomethane, methylene bromide
CAS Registry No: 74-95-3
Molecular Formula: CH₂Br₂
Molecular Weight: 173.835
Melting Point (°C):
-52.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
97.0 (Horvath 1982; Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
2.4970, 2.4842 (20°C, 25°C, Dreisbach 1961)
2.4970 (Horvath 1982; Weast 1982–83)
Molar Volume (cm³/mol):
70.1 (Stephenson & Malanowski 1987)
76.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
11480* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
11700, 11930 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
11486 (Seidell 1940; quoted, Deno & Berkheimer 1960)
17500 (shake flask-residue volume method, Booth & Everson 1948)
11000 (O’Connell 1963; Jolles 1966)
11442* (summary of literature data, Horvath 1982)
11500 (Dean 1985)
12800*, 11400 (19.3°C, 29.5°C, shake flask-GC/TC, measured range 0–90.1°C, Stephenson 1992)
11420, 12030, 12270, 12580 (20, 30, 35, 40°C, infinite dilution activity coeff. \( \gamma \)-GC, Tse et al. 1992)
11114, 12060, 13052 (20, 30, 40°C, activity coeff. \( \gamma \)-differential pressure transducer, Wright et al. 1992)
12300 (20°C, limiting activity coeff. \( \gamma \) by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4626, 7518 (20°C, 30°C, Rex 1906)
5775* (Antoine eq. regression, temp range –35.1 to 98.6°C, Stull 1947)
6034 (calculated by formula, Dreisbach 1961)

\[
\log (P/\text{mmHg}) = 7.0625 – 1327.8/(220.58 + t/°C); \text{temp range 17–236°C (Antoine eq., Dreisbach 1961)}
\]

5767 (calculated-Antoine eq., Weast 1972–73)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 8722.0/(T/K)] + 8.028019; \text{temp range –35.1 to 98.6°C (Antoine eq., Weast 1972–73)}
\]

5922 (Antoine eq. regression, Kudchadker et al. 1979)
\[
\log (P/\text{mmHg}) = 7.82594 – 1784.9/(263.73 + t°C) \text{(Antoine eq., Kudchadker et al. 1979)}
\]
6034 (calculated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/\text{kPa}) = 6.1874 – 1327.8/(-52.57 + T/K); \text{temp range 290–409 K (Antoine eq., Stephenson & Malanowski 1987)}
\]
Halogenated Aliphatic Hydrocarbons

log (P/mmHg) = 35.3525 – 3.0445 × 10^3/(T/K) – 9.5792·log (T/K) + 5.8258 × 10^{-10}·(T/K) + 2.9443 × 10^{-6}·(T/K)^2; temp range 221–611 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated):
90.0 (calculated-1/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)
73.16 (calculated-bond method, Hine & Mookerjee 1975)
86.13 (batch stripping-GC, Nicholson et al. 1984)
86.03 (Munz & Roberts 1989)
70.9, 111.5, 142, 172 (20, 30, 35, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)
72.7, 141, 252 (20, 30, 40°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
281, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
25.4, 48.3, 81.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

ln K_{AW} = 11.70 – 4418/(T/K); seawater of salinity of 30.4‰, temp range 0–20°C (Moore et al. 1995)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:
2.50 (Hansch et al. 1968)
1.70 (recommended, Sangster 1993)
1.70 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
1.70, 1.65, 1.64 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
3.07 (head-space GC, Abraham et al. 2001)

Biodegradation:
k = 2.1 × 10^{-4} min^{-1} with t_{1/2} = 24 min in anoxic sediment-water suspension (Jafvert & Wolfe 1987)
**Biotransformation:**

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

**Half-Lives in the Environment:**

Air: disappearance tₜ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

- estimated as toxic chemical residence time of 46 d with rate constant of 2.5 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for the reaction with OH radical at 300 K (Singh et al. 1980);
- photooxidation tₜ = 851–8510 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: tₜ = 183 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)
- tₜ = 55 h in anoxic sediment-water suspension (Jafvert & Wolfe 1987);
- tₜ = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
- measured k ≤ 0.005 M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 2 and 21°C, with tₜ ≥ 80 d at pH 7 (Yao & Haag 1991).

Ground water: tₜ = 336–1344 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: tₜ = 55 h in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

**Soil:** tₜ = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

**Biota:**

### TABLE 5.1.2.2.1

**Reported aqueous solubilities of dibromomethane at various temperatures**

\[
S/(\text{wt}) = 1.1594 - 4.3267 \times 10^{-3}(t/\text{°C}) + 1.8201 \times 10^{-4}(t/\text{°C})^2 - 1.3335 \times 10^{-6}(t/\text{°C})^3 \quad (1)
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Rex 1906</th>
<th>Horvath 1982</th>
<th>Stephenson 1992</th>
<th>Tse et al. 1992</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>volumetric method</td>
<td>summary of literature data</td>
<td>shake flask-GC</td>
<td>activity coefficient</td>
</tr>
<tr>
<td>0</td>
<td>11730</td>
<td>5 11594</td>
<td>0 11700</td>
<td>20 11420</td>
</tr>
<tr>
<td>10</td>
<td>11460</td>
<td>10 11330</td>
<td>9.7 11300</td>
<td>30 12030</td>
</tr>
<tr>
<td>20</td>
<td>11480</td>
<td>20 11350</td>
<td>19.3 12800</td>
<td>35 12270</td>
</tr>
<tr>
<td>30</td>
<td>11760</td>
<td>25 11442</td>
<td>29.5 11400</td>
<td>40 12580</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gross &amp; Saylor 1931</th>
<th>activity coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-interferometer</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>15</td>
<td>11700</td>
</tr>
<tr>
<td>30</td>
<td>11930</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
FIGURE 5.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.2
Reported vapor pressures of dibromomethane at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P/\text{Pa}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>–35.1</td>
<td>133.3</td>
</tr>
<tr>
<td>–13.2</td>
<td>666.6</td>
</tr>
<tr>
<td>–2.40</td>
<td>1333</td>
</tr>
<tr>
<td>9.70</td>
<td>2666</td>
</tr>
<tr>
<td>23.3</td>
<td>5333</td>
</tr>
<tr>
<td>31.6</td>
<td>7999</td>
</tr>
<tr>
<td>42.3</td>
<td>13332</td>
</tr>
<tr>
<td>58.5</td>
<td>26664</td>
</tr>
<tr>
<td>79.0</td>
<td>53329</td>
</tr>
<tr>
<td>98.6</td>
<td>101325</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–52.8</td>
</tr>
</tbody>
</table>
**TABLE 5.1.2.2.3**

Reported Henry’s law constants of dibromomethane at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \quad (1)
\]

\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2)
\]

\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)
\]

\[
\ln H = A - B/(T/K) \quad (4)
\]

\[
K_{AW} = A - B(1/K) + C(1/K)^2 \quad (5)
\]

Tse et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>70.9</td>
</tr>
<tr>
<td>30</td>
<td>111.5</td>
</tr>
<tr>
<td>35</td>
<td>142</td>
</tr>
<tr>
<td>40</td>
<td>172</td>
</tr>
</tbody>
</table>

Wright et al. 1992

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>72.7</td>
</tr>
<tr>
<td>30</td>
<td>141</td>
</tr>
<tr>
<td>40</td>
<td>252</td>
</tr>
</tbody>
</table>

Bhatia & Sandler 1995

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>281</td>
</tr>
<tr>
<td>50</td>
<td>513</td>
</tr>
</tbody>
</table>

Moore et al. 1995

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>25.4</td>
</tr>
<tr>
<td>10</td>
<td>48.3</td>
</tr>
<tr>
<td>20</td>
<td>81.9</td>
</tr>
</tbody>
</table>

**Activity Coefficient**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>eq. 1</td>
<td>K_{AW}</td>
</tr>
<tr>
<td>A</td>
<td>11.70 ± 0.03</td>
</tr>
<tr>
<td>B</td>
<td>4418 ± 154</td>
</tr>
</tbody>
</table>

**Gas Stripping-GC**

seawater, salinity 30.4‰
FIGURE 5.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for dibromomethane.
5.1.2.3 Tribromomethane

Common Name: Tribromomethane
Synonym: bromoform, methenyl tribromide
Chemical Name: tribromomethane
CAS Registry No: 75-25-2
Molecular Formula: CHBr3
Molecular Weight: 252.731
Melting Point (°C):
8.69 (Lide 2003)
Boiling Point (°C):
149.1 (Lide 2003)
Density (g/cm³ at 20°C):
2.8910 (Kahlbaum & Arndt 1898; Riddick et al. 1986)
2.8917, 2.8909 (Kudchadker et al. 1979)
Molar Volume (cm³/mol):
87.42 (20°C, calculated-density)
99.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
3010, 3190 (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)
3110 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
3190 (30°C, Seidell 1941)
3033 (Verschueren 1977)
3100 (recommended, Horvath 1982)
3931 (30°C, headspace-GC, McNally & Grob 1984)
3200 (30°C, Dean 1985)
3180 (30°C, selected, Riddick et al. 1986)
3235, 3452, 3695 (20, 30, 40°C, infinite dilution activity coeff. $\gamma$-GC, Tse et al. 1992)
3978, 4555, 3467 (20, 35, 50°C, activity coeff. $\gamma$-differential pressure transducer, Wright et al. 1992)
3163 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
667* (22°C, summary of literature data, temp range 22–150.5°C, Stull 1947)
2453* (47.207°C, temp range 47.207–139.055°C, Boublík & Aim 1972; quoted, Boublík et al. 1984)
815 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9673.3/(T/K)] + 7.875367; temp range 22–150°C (Antoine eq., Weast 1972–73)
715 (calculated-Antoine eq., Boublík et al. 1973)
log (P/mmHg) = 6.82182 – 1376.748/(200.966 + t°C); temp range 30–100°C (Antoine eq. from reported expn. data, Boublík et al. 1973)
720 (calculated-Antoine eq., Kudchadker et al. 1979)
log (P/mmHg) = 7.03141 – 1511.50/(214.21 + t°C) (Antoine eq., Kudchadker et al. 1979)
717 (calculated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 5.97839 – 1294.382/(202.729 + t°C); temp range 30–100.8°C (Antoine eq. from reported expn. data, Boublík et al. 1984)
log (P/mmHg) = 6.8218 – 1376.7/(201.0 + t°C); temp range 30–101°C (Antoine eq., Dean 1985, 1992)
790 (quoted, Riddick et al. 1986)
727 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = -10.2943 – 2.170 × 10^3/(T/K) + 9.1193·log (T/K) – 1.6495 × 10^-2·(T/K) + 7.4917 × 10^-6·(T/K)^2;
temp range 281–696 K (vapor pressure eq., Yaws 1994)
685.5 (selected and summary of literature data, temp range 281.2–478.15 K, Xiang 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
68.3 (calculated-1/K_{AW}, C_W/C_A, Hine & Mookerjee 1975)
7.66 (calculated-bond method, Hine & Mookerjee 1975)
62.3, 62.0 (calculated-P/C, recommended, Mackay & Shiu 1981,1990)
56.7 (20°C, calculated-P/C, Mabey et al. 1982)
43.6, 43.6; 58.8 (20°C, batch stripping-GC, calculated-P/C, distilled water, Nicholson et al. 1984)
46.6, 41.54, 43.6 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
ln [H/(atm m^3/mol)] = 116.0 – 5670/(T/K); temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)
54.2 (EPICS-LSC, Munz & Roberts 1987, 1989)
log K_{AW} = 4.729 – 1905/(T/K); temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)
53.9 (gas stripping-GC, Warner et al. 1987)
56.7 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
40.5, 70.9, 122 (20, 30, 40°C, infinite dilution activity coeff. γ∞-GC, Tse et al. 1992)
34.0, 71.6, 207 (20, 35, 50°C, activity coeff. γ∞-differential pressure transducer, Wright et al. 1992)
43.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
182, 536 (10, 20°C, gas stripping-GC, Moore et al. 1995)
14.3, 29.2, 52.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

ln K_{AW} = 13.16 – 4973/(T/K); seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)

2.30 (calculated as per Tute 1971, Callahan et al. 1979)
2.38 (calculated-f const., Mabey et al. 1982; Valsaraj 1988)
2.67 (recommended, Hansch et al. 1979)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization: calculated t_{1/2} = 63 min to 24.2 d (using Langbein & Durum 1967 published O_{2} reaeration values)
and t_{1/2} = 65.6 d both from rivers and streams (Kaczmar et al. 1984).
Photolysis: photocatalyzed mineralization by the presence of TiO_{2} with the rate of 6.2 ppm/min per gram of
catalyst (Ollis 1985).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
with NO_{3} radical and k_{O3} with O_{3} or as indicated, *data at other temperatures and/or the Arrhenius expression
see reference:
k << 360 M^{-1} h^{-1} for singlet oxygen and k = 0.5 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)
photooxidation $t_{1/2} = 1299–12989$ h, based on estimated rate constant for the reaction with OH radical in air 
(Atkinson 1987; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7$ M$^{-1}$ s$^{-1}$ for reaction with OH radical in water with reference to CH$_3$CCl$_3$ (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{\text{OH(aq.)}} = (1.3 \pm 0.6) \times 10^8$ M$^{-1}$ s$^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: a maximum $t_{1/2} = 686$ yr has been estimated at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977) which corresponds to a first-order rate constant $k = 3.2 \times 10^{-11}$ s$^{-1}$ (Radding et al. 1977; Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard et al. 1991);

rate constant $k = 3.2 \times 10^{-11}$ s$^{-1}$ with $t_{1/2} = 686$ yr at pH 7 and 25°C (Mabey & Mill 1978)

rate constant $k = 2.5 \times 10^{-9}$ h$^{-1}$ assigned by analogy to trichloromethane (Mabey et al. 1982).

Biodegradation: $t_{1/2} = 672–4320$ h in soil, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991);

anaerobic $t_{1/2} = 2688–17280$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant $k \sim 1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$\text{t}_{1/2} = 1299–12989$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 686$ yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water: $t_{1/2} = 1344–8640$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672–4320$ h, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 5.1.2.3.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities of tribromomethane at various temperatures</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gross &amp; Saylor 1931</th>
<th>Tse et al. 192</th>
<th>Wright et al. 1992</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>shake flask-interferometer</strong></td>
<td><strong>activity coefficient</strong></td>
<td><strong>activity coefficient</strong></td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m$^{-3}$</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>15</td>
<td>3010</td>
<td>20</td>
</tr>
<tr>
<td>30</td>
<td>3190</td>
<td>30</td>
</tr>
<tr>
<td>40</td>
<td>3695</td>
<td>40</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
Halogenated Aliphatic Hydrocarbons

**FIGURE 5.1.2.3.1** Logarithm of mole fraction solubility (ln $x$) versus reciprocal temperature for tribromomethane.

**TABLE 5.1.2.3.2**
Reported vapor pressures of tribromomethane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1)
\]

\[
\ln P = A - \frac{B}{T/K} \quad (1a)
\]

\[
\log P = A - \frac{B}{C + T/K} \quad (2)
\]

\[
\ln P = A - \frac{B}{C + T/K} \quad (2a)
\]

\[
\log P = A - \frac{B}{C + t/°C} \quad (3)
\]

\[
\ln P = A - \frac{B}{C + t/°C} \quad (3a)
\]

\[
\log P = A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th>Kireev &amp; Simnikow 1941</th>
<th>Stull 1947</th>
<th>Boublik &amp; Aim 1972</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>in Boublik et al. 1984</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>in Boublik et al. 1984</strong></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>30.0</td>
<td>987</td>
<td>47.207</td>
</tr>
<tr>
<td>35.0</td>
<td>1267</td>
<td>59.767</td>
</tr>
<tr>
<td>40.0</td>
<td>1747</td>
<td>69.518</td>
</tr>
<tr>
<td>50.0</td>
<td>2946</td>
<td>76.389</td>
</tr>
<tr>
<td>60.0</td>
<td>4693</td>
<td>82.821</td>
</tr>
<tr>
<td>70.0</td>
<td>7399</td>
<td>87.709</td>
</tr>
<tr>
<td>80.0</td>
<td>11306</td>
<td>93.356</td>
</tr>
<tr>
<td>90.0</td>
<td>16852</td>
<td>98.173</td>
</tr>
<tr>
<td>110.0</td>
<td>24198</td>
<td>103.595</td>
</tr>
<tr>
<td></td>
<td></td>
<td>108.003</td>
</tr>
<tr>
<td></td>
<td></td>
<td>113.216</td>
</tr>
<tr>
<td>mp/°C</td>
<td>8.5</td>
<td>118.078</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
FIGURE 5.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for tribromomethane.
5.1.2.4 Bromoethane (Ethyl bromide)

\[ Br \]

Common Name: Ethyl bromide
Synonym: bromoethane, monobromoethane
Chemical Name: ethyl bromide, bromoethane
CAS Registry No: 74-96-4
Molecular Formula: C₂H₅Br, CH₃CH₂Br
Molecular Weight: 108.965
Melting Point (°C):
\(-118.60\) (Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
38.5 (Lide 2003)
Density (g/cm³ at 20°C):
1.4594, 1.4492 (20°C, 25°C, Dreisbach 1959)
1.4505 (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
75.12 (calculated from density)
75.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
27.55, 26.48 (25°C, at bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
5.858 (quoted, Riddick et al. 1986)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
9140* (20°C volumetric method, measured range 0–30°C, Rex 1906)
9600 (17.5°C, volumetric method, Fühner 1924)
8880 (30°C, van Arkel & Vles 1936)
9064 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
9000 (shake flask-interferometry, Donahue & Bartell 1952)
8939* (summary of literature data, temp range 0–30°C, Horvath 1982)
9100 (Dean 1985; Riddick et al. 1986)
9000* (tentative value, temp range 0–°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

\[ S/(wt\%) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/K) + 1.29448 \times 10^{-4} \cdot (T/K)^2, \] temp range 273–303 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
51440, 75140 (20°C, 30°C, Rex 1906)
53329* (21°C, summary of literature data, temp range –74.3 to 38.4°C, Stull 1947)
62460 (calculated-Antoine eq., Dreisbach 1959)
\[ \log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/°C); \] temp range –32 to 110°C (Antoine eq. for liquid state, Dreisbach 1959)
\[ \log (P/mmHg) = 6.91995 - 1090.810/(231.71 + t/°C); \] pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
\[ \log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277; \] temp range 74.3 to 229.5°C (Antoine eq., Weast 1972–73)
62230 (extrapolated-Antoine eq., Boublik et al. 1984)
\[ \log (P/kPa) = 6.11352 - 1121.957/(234.741 + t/°C); \] temp range 28.145–75.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9886 – 1121.9/(234.7 + t°C); temp range 28–75°C (Antoine eq., Dean 1985, 1992)
62470  (lit; average, Riddick et al. 1986)
log (P/kPa) = 6.04485 – 1090.81/(231.71 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
62470  (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.66835 – 1090.81/(–41.44 + T/K); temp range 334–504 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.77490 – 1602.405/(12.999 + T/K); temp range 326–454 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.99873 – 1619.697/(T/K); temp range 452–503 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 3.81816 – 2.517×10³/(T/K) – 10.329·log (T/K) – 2.3368×10⁻¹¹·(T/K) + 5.4956×10⁻⁶·(T/K)²;
temp range 155–504 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
766  (calculated-1/Kₜ₍, Cₜ/Cₜ, reported as exptl., Hine & Mookerjee 1975)
751  (computed value, Yaws et al. 1991)
767  (γ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log Kₜ₃₉:
1.60  (calculated-π const., Hanch et al. 1968)
1.61  (shake flask-GC, Hanch et al. 1975; Hansh & Leo 1979, 1987)
1.61  (recommended, Sangster 1989)
1.61  (recommended, Hanch et al. 1995)

Octanol/Air Partition Coefficient, log Kₜ₃₉ at 25°C:
1.53  (calculated-measured γ from pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Kₜ₉:

Environmental Fate Rate Constants, k and Half-Lives, tᵯ:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: k = 2.64×10⁻⁷ s⁻¹ with tᵯ = 30 d at pH 7 and 25°C (Mabey & Mill 1978)
   k = 9.4×10⁻⁴ h⁻¹ at pH 7 and 25°C with tᵯ = 30 d (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (kᵣ) and Elimination (kₑ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: disappearance tᵯ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976),
Surface water: tᵯ = 30 d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)
### TABLE 5.1.2.4.1
Reported aqueous solubilities of bromoethane at various temperatures

\[
S/(\text{wt%}) = 1.0557 - 0.01309 \cdot (t/°C) + 3.3850 \times 10^{-4} \cdot (t/°C)^2 - 2.950 \times 10^{-6} \cdot (t/°C)^3 \quad (1)
\]

\[
S/(\text{wt%}) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/K) + 1.29448 \times 10^{-4} \cdot (T/K)^2 \quad (2)
\]

<table>
<thead>
<tr>
<th>Rex 1906 volumetric method</th>
<th>Horvath 1982 summary of literature data</th>
<th>Horvath &amp; Getzen 1999 tentative, IUPAC-NIST</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
</tr>
<tr>
<td>------</td>
<td>---------</td>
<td>------</td>
</tr>
<tr>
<td>0</td>
<td>10670</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>9650</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>9140</td>
<td>20</td>
</tr>
<tr>
<td>30</td>
<td>8960</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
</tr>
<tr>
<td>eq. 1 S/wt%</td>
<td>eq. 2 S/wt%</td>
<td>experi</td>
</tr>
<tr>
<td></td>
<td></td>
<td>tem range 273–303 K</td>
</tr>
</tbody>
</table>

**FIGURE 5.1.2.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromoethane.
TABLE 5.1.2.4.2
Reported vapor pressures of bromoethane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \\
\log P &= A - \frac{B}{C + t/^\circ C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/^\circ C} \\
\log P &= A - \frac{B}{T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>t/^\circ C</th>
<th>Zmaczynski 1930</th>
<th>Stull 1947</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P/Pa</td>
<td>t/^\circ C</td>
</tr>
<tr>
<td>28.145</td>
<td>70095</td>
<td>–74.3</td>
</tr>
<tr>
<td>33.247</td>
<td>83515</td>
<td>–56.4</td>
</tr>
<tr>
<td>43.560</td>
<td>120803</td>
<td>–47.5</td>
</tr>
<tr>
<td>48.771</td>
<td>143268</td>
<td>–37.8</td>
</tr>
<tr>
<td>54.018</td>
<td>169066</td>
<td>–26.7</td>
</tr>
<tr>
<td>59.300</td>
<td>198543</td>
<td>–19.5</td>
</tr>
<tr>
<td>64.619</td>
<td>232113</td>
<td>–10.0</td>
</tr>
<tr>
<td>69.94</td>
<td>270150</td>
<td>4.50</td>
</tr>
<tr>
<td>75.365</td>
<td>312960</td>
<td>21.0</td>
</tr>
</tbody>
</table>

mp/^\circ C = –117.8

FIGURE 5.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for bromoethane.
5.1.2.5 1,2-Dibromoethane

\[ \text{Br} - \text{Br} \]

Common Name: 1,2-Dibromoethane
Synonym: ethylene bromide, ethylene dibromide, sym-dibromoethane, EDB
Chemical Name: 1,2-dibromoethane
CAS Registry No: 106-93-4
Molecular Formula: C₂H₄Br₂, CH₂BrCH₂Br
Molecular Weight: 187.861
Melting Point (°C):
9.84 \text{ (Lide 2003)}
Boiling Point (°C):
131.6 \text{ (Lide 2003)}
Density (g/cm³ at 20°C):
2.1792, 2.1688 \text{ (20°C, 25°C, Dreisbach 1959; Horvath 1982)}
2.1791, 2.1687 \text{ (20°C, 25°C, Riddick et al. 1986)}
Molar Volume (cm³/mol):
86.25 \text{ (20°C, calculated-density, Stephenson & Malanowski 1987)}
98.4 \text{ (calculated-Le Bas method at normal boiling point)}
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
41.73, 36.35 \text{ (25°C, at bp, Riddick et al. 1986)}
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
10.03 \text{ (calculated, Dreisbach 1959)}
10.945 \text{ (quoted, Riddick et al. 1986)}
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
3920, 4310 \text{ (15°C, 30°C, shake flask-interferometer, Gross & Saylor 1931)}
4040* \text{ (measured range 0–50°C, van Arkel & Vles 1936)}
4017 \text{ (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)}
8600 \text{ (shake flask-volumetric method, Booth & Everson 1948)}
4200 \text{ (measured by Dow Chemical, Dreisbach 1959)}
3510* \text{ (20°C, shake flask-GC, measured range 3–34°C, Chiu & Freed 1977)}
2910 \text{ (shake flask-GC, Jones et al. 1977/78)}
3520 \text{ (shake flask-GC, Chiu et al. 1979)}
4320, 4321 \text{ (20°C, 25°C, shake flask-GC, Mackay et al. 1980)}
4152* \text{ (summary of literature data, Horvath 1982)}
4310 \text{ (30°C, Verschueren 1983)}
4290 \text{ (30°C, selected, Riddick et al. 1986)}
3120 \text{ (shake flask-reverse phase polarography, Tokoro et al. 1988)}
4120*, 4310 \text{ (19.5°C, 30.7°C, shake flask-GC/TC, measured range 10.0–90.6°C, Stephenson 1992)}
4192 \text{ (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)}
3910* \text{ (tentative value, temp range 0–75°C. IUPAC-NIST Solubility Data Series, Hovath & Getzen 1999a)}
S/(wt%) = 3.8651 – 2.7921 \times 10^{-2} \cdot (T/K) + 5.45647 \times 10^{-5} \cdot (T/K)^2, \text{ temp range 273–348 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)}

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1333 \text{ (18.2°C, summary of literature data, temp range –27 to 131.1°C, Stull 1947)}
1560 \text{ (calculated-Antoine eq., Dreisbach 1959)}
\log (P/mmHg) = 7.06245 – 1469.7/(220.0 + t°C); \text{ temp range 43–215°C (Antoine eq. for liquid state, Dreisbach 1959)}
log (P/mmHg) = \[-0.2185 \times 9229.4/(T/K)\] + 7.93581; temp range –27 to 304°C (Antoine eq., Weast 1972–73)
1466, 2266 (20°C, 30°C, Verschueren 1983)
1626 (interpolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 5.62666/(1156.346 + t/°C); temp range 52.56–131.41°C (Antoine eq. from reported
exptl. data, Boublík et al. 1984)
log (P/mmHg) = 6.72148 – 1280.82/(201.75 + t/°C); temp range 52–131°C (Antoine eq., Dean 1985, 1992)
1540 (lit. average, Riddick et al. 1986)
log (P/kPa) = 4.32297 – 1156.3/(230.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 10.03 – 2863/(T/K); temp range 228–248 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 9.009 – 2606.5/(T/K); temp range 251–281 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 7.501 – 2181.1/(T/K); temp range 283–317 K (liquid, Antoine eq.-III, Stephenson & Malanowski
1987)
log (P/kPa) = 6.18375 – 1469.7/(–53.15 + T/K); temp range 316–488 K (Antoine eq.-IV, Stephenson &
Malanowski 1987)
log (P/kPa) = 6.16941 – 3200/(117.25 + T/K); temp range 404–578 K (Antoine eq.-V, Stephenson &
Malanowski 1987)

log (P/mmHg) = 16.8759 – 2.4267 \times 10^3/(T/K) – 3.0891 \times 10^{-10}\cdot(T/K)^2; temp range 283–650 K (vapor pressure
eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C):

71.49 (calculated as 1/K_AW, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
15.64, 110.7 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
65.86* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm m3 mol–1)] = 5.703 – 3876/(T/K); temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
71.49, 133.12 (quoted, calculated-QSAR, Nirmalakhandan & Speece 1988)
83.07 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
70.77 (computed value, Yaws et al. 1991)
52.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
52.02 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
54.84 (20°C, selected from reported experimental determined values, Staudeinger & Roberts 2001)
log K_AW = 3.661 – 1556/(T/K) (summary of literature data, Staudeinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_OW:

1.96 (shake flask, Log P Database, Hansch & Leo 1987)
1.96 (recommended, Sangster 1994)
1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
0.301 (calculated-K_OC as per Kenaga & Goring 1978, Kenaga 1980)

Sorption Partition Coefficient, log K_OC:

1.556 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
1.643 (soil, quoted, Kenaga 1980; Kenaga & Goring 1980)
1.699 (soil, calculated as per Kenaga & Goring 1978, Kenaga 1980)
1.643 (soil, selected, Jury et al. 1990)
1.64 (soil, organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k and Half-Lives, t_1/2:

Volatileization: estimated volatilization t_1/2 ~ 6.1 h from water (Thomas 1982)
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 296 K (discharge flow system, Howard & Evenson 1976)
Halogenated Aliphatic Hydrocarbons

\[ k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{\text{OH}}(\text{obs.}) = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \] (SAR [structure-activity relationship], Atkinson 1985)

\[ k_{\text{OH}} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of 0.01 d}^{-1}, \quad k_{\text{O3}} < 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of <6 \times 10^{-7} d}^{-1} \text{ at room temp.} \] (Atkinson 1985)

\[ k_{\text{O3(aq.)}} \leq 0.014 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 2 and 22°C, with a half-life of 28 d at pH 7} \] (Yao & Haag 1991).

Hydrolysis: EDB hydrolyzes to ethylene glycol and bromoethanol in water at pH 7 and 25°C with \( t_{\text{v}} = 5–10 \text{ d} \) (Leinster et al. 1978; quoted, Verschueren 1983);

\[ k = 9.9 \times 10^{-6} \text{ h}^{-1} \text{ at pH 7 and 25°C with a calculated } t_{\text{v}} = 8.0 \text{ yr} \] (Jungclaus & Cohen 1986; quoted, Ellington 1989);

rate constant \( k = (8.9 \pm 0.1) \times 10^{-9} \text{ s}^{-1} \text{ in water at 25°C and pH 7.5 with an estimated half-life of 2.5 yr} \) (Vogel & Reinhard 1986);

\[ t_{\text{v}} = 2.2 \text{ yr, based on measured neutral hydrolysis rate constant at pH 7 and 25°C} \] (Weintraub et al. 1986; quoted, Howard et al. 1991).

Biodegradation: aerobic \( t_{\text{v(aq.)}} = 672–4320 \text{ h, based on unacclimated aqueous aerobic biodegradation screening} \)

\[ \text{test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991); } \]

anaerobic \( t_{\text{v(aq.)}} = 48–360 \text{ h, based on anaerobic stream and pond water sediment die-away test data (Jafvert & Wolfe 1987; quoted, Howard et al. 1991).} \)

Biotransformation:

Bioconcentration, Uptake (\( k_{1} \)) and Elimination (\( k_{2} \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance \( t_{\text{v}} = 2.4–24 \text{ h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); } \)

\[ \text{photooxidation } t_{\text{v}} = 257–2567 \text{ h, based on estimated rate constant for the reaction with hydroxyl} \]

\[ \text{radical in air (Atkinson 1987; quoted, Howard et al. 1991).} \]

Surface water: \( t_{\text{v}} = 672–4320 \text{ h, based on unacclimated aqueous aerobic biodegradation (Howard et al. 1991); } \)

\[ k(\text{exptl}) \leq 0.014 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 2 and 22°C, with } t_{\text{v}} \geq 28 \text{ d at pH 7} \] (Yao & Haag 1991).

Ground water: \( t_{\text{v}} = 470–2880 \text{ h, based on data from anaerobic ground water ecosystem study (Wilson et al. 1986; quoted, Howard et al. 1991); } \)

data from an aerobic ground water ecosystem study (Swindoll et al. 1987; quoted, Howard et al. 1991).

Sediment: calculated \( t_{\text{v}} = 1500 \text{ d at 25°C and pH 7, based on studies in pure water and in barely saturated} \)

\[ \text{subsurface sediment at 25–60°C (Haag & Mill 1988).} \]

Soil: estimated \( t_{\text{v}} \sim 3650 \text{ d of volatilization loss from soil (Jury et al. 1990); } \)

\[ \text{disappearance } t_{\text{v}} < 2.0 \text{ d, estimated from the volatilization loss of mixtures (Anderson et al. 1991); } \]

\[ t_{\text{v}} = 672–4320 \text{ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).} \]

Biota:

### TABLE 5.1.2.5.1

Reported aqueous solubilities of 1,2-dibromoethane at various temperatures

\[
S/(\text{wt}) = 0.36583 + 1.4836 \times 10^{-1}(T/°C) + 3.48175 \times 10^{-6}(T/°C)^2 + 6.47685 \times 10^{-7}(T/°C)^3 \quad (1)
\]

\[
S/(\text{wt}) = 3.8651 - 2.7921 \times 10^{-2}(T/K) + 5.45647 \times 10^{-5}(T/K)^2 \quad (2)
\]

1.

<table>
<thead>
<tr>
<th>Gross &amp; Saylor 1931</th>
<th>van Arkel &amp; Vles 1936</th>
<th>Chiou &amp; Freed 1977</th>
<th>Horvath 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-interferometer</td>
<td>shake flask-GC</td>
<td>summary of literature data</td>
<td></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g.m}^{-3} )</td>
<td>( t/°C )</td>
<td>( S/\text{g.m}^{-3} )</td>
</tr>
<tr>
<td>15</td>
<td>3920</td>
<td>0</td>
<td>3340</td>
</tr>
<tr>
<td>30</td>
<td>4310</td>
<td>20</td>
<td>4020</td>
</tr>
<tr>
<td>45</td>
<td>4900</td>
<td>35</td>
<td>4490</td>
</tr>
<tr>
<td>50</td>
<td>5290</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
### TABLE 5.1.2.5.1 (Continued)

<table>
<thead>
<tr>
<th>Gross &amp; Saylor 1931</th>
<th>van Arkel &amp; Vles 1936</th>
<th>Chiou &amp; Freed 1977</th>
<th>Horvath 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-interferometer</td>
<td>shake flask-GC</td>
<td>summary of literature data</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>30</td>
<td>4310</td>
<td>40</td>
<td>4722</td>
</tr>
<tr>
<td>50</td>
<td>5780</td>
<td>70</td>
<td>7089</td>
</tr>
</tbody>
</table>

#### 2.

<table>
<thead>
<tr>
<th>Stephenson 1992</th>
<th>Horvath &amp; Getzen 1999a</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC</td>
<td>tentative, IUPAC-NIST</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>10.1</td>
<td>3950</td>
</tr>
<tr>
<td>19.5</td>
<td>4120</td>
</tr>
<tr>
<td>30.7</td>
<td>4310</td>
</tr>
<tr>
<td>39.6</td>
<td>4440</td>
</tr>
<tr>
<td>50</td>
<td>4930</td>
</tr>
<tr>
<td>59.9</td>
<td>4890</td>
</tr>
<tr>
<td>70.2</td>
<td>5420</td>
</tr>
<tr>
<td>75</td>
<td>5950</td>
</tr>
<tr>
<td>80</td>
<td>6430</td>
</tr>
</tbody>
</table>

#### FIGURE 5.1.2.5.1

Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2-dibromomethane.
### TABLE 5.1.2.5.2
Reported Henry's law constants of 1,2-dibromoethane at various temperatures

**Ashworth et al. 1988**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>30.4</td>
</tr>
<tr>
<td>15</td>
<td>48.6</td>
</tr>
<tr>
<td>20</td>
<td>61.8</td>
</tr>
<tr>
<td>25</td>
<td>65.9</td>
</tr>
<tr>
<td>30</td>
<td>81.1</td>
</tr>
</tbody>
</table>

\[
\ln \left( \frac{H}{\text{atm} \cdot \text{m}^3/\text{mol}} \right) = A - \frac{B}{T/\text{K}}
\]

A 5.703

B 3876

### FIGURE 5.1.2.5.2
Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dibromomethane.
5.1.2.6 1-Bromopropane

Common Name: 1-Bromopropane
Synonym: bromopropane, monobromopropane, n-propyl bromide, propyl bromide
Chemical Name: n-propyl bromide, 1-bromopropane
CAS Registry No: 106-94-5
Molecular Formula: C₃H₇Br, CH₃CH₂CH₂Br
Molecular Weight: 122.992

Melting Point (°C):
-110.3 (Lide 2003)

Boiling Point (°C):
71.1 (Lide 2003)

Density (g/cm³ at 20°C):
1.3536, 1.3452 (20°C, 25°C, Dreisbach 1961)
1.3537 (Horvath 1982)

Molar Volume (cm³/mol):
90.86 (20°C, calculated-density)
97.30 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
31.88, 68.8 (25°C, 68.8°C, Riddick et al. 1986)

Enthalpy of Fusion, ΔHfus (kJ/mol):
9.037 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2450* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
2275 (19.5°C, shake flask, Fühner 1924)
2310 (30°C, shake flask-interferometer, Gross & Saylor 1931)
2312 (30°C, shake flask, Van Arkel & Vles 1936)
2454 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
2460 (calculated-Kow, Hansch et al. 1968)
2450 (20°C, expl., Korenman et al. 1971)
2427* (summary of literature data, Horvath 1982)
2300 (30°C, Dean 1985; Riddick et al. 1986)
2340* (tentative value, IUPAC-NIST Solubility Data Series, temp range 0–30°C Horvath & Getzen 1999)

\[ S/(wt\%) = 9.0608 - 0.05911 \times (T/K) + 9.8925 \times 10^{-5} \times (T/K)^2 \], temp range 273–303 K (Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14770, 22740 (20°C, 30°C, volumetric method Rex 1906)
13332* (18°C, summary of literature data, temp range –53.0 to 71°C, Stull 1947)
18440 (calculated by formula, Dreisbach 1961)

\[ \log (P/mmHg) = 6.91065 - 1194.889/(225.51 + t/°C) \], temp range –6 to 107°C (Antoine eq. for liquid state, Dreisbach 1961)

\[ \log (P/mmHg) = 6.91065 - 1194.889/(225.51 + t/°C) \], pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

18300 (interpolated-Antoine eq., Boublík et al. 1984)

\[ \log (P/kPa) = 6.09224 - 1232.529/(230.19 + t/°C) \], temp range 0–30°C (Antoine eq. from reported explt. data of Rex 1906, Boublík et al. 1984)

18440 (selected, Riddick et al. 1986)

\[ \log (P/kPa) = 6.03960 - 1194.33/(225.22 + t/°C) \], temp range not specified (Antoine eq., Riddick et al. 1986)
log \( (P/L \text{ kPa}) = 6.03555 - 1194.889/(47.64 + T/K) \); temp range 250–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \( (P/L \text{ kPa}) = 6.03823 - 1193.612/(48.005 + T/K) \); temp range 301–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( (P/mmHg) = -9.0284 - 1.8916 \times 10^3/(T/K) + 9.691 \log (T/K) - 2.7013 \times 10^{-2} \cdot (T/K)^2 \); temp range 163–544 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):

- 964.4 (calculated-1/K\(_{AW}\), C\(_A\)/C\(_W\), reported as exptl., Hine & Mookerjee 1975)
- 1133, 1564 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 766.0 (calculated-QSAR, Nirmalakhandan & Speece 1988)
- 732 (computed value, Yaws et al. 1991)
- 950 (\( \gamma^\infty \) from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 2.10 (shake flask-GC, Fujita et al. 1964; Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
- 2.10 (recommended, Sangster 1989, 1993)
- 2.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: \( k = 3.04 \times 10^{-7} \text{ s}^{-1} \) with estimated \( t_{1/2} = 26 \text{ d} \) at pH 7 and 25°C (Mabey & Mill 1978)

\( k = 1.1 \times 10^{-3} \text{ h}^{-1} \) at pH 7 and 25°C with estimated \( t_{1/2} = 26 \text{ d} \) (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k\(_1\)) and Elimination (k\(_2\)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance \( t_{1/2} = 2.4–24 \text{ h} \) from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated \( t_{1/2} = 26 \text{ d} \) at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:
### TABLE 5.1.2.6.1
Reported aqueous solubilities of 1-bromopropane at various temperatures

\[
S/(\text{wt%}) = 0.2971 - 0.04225 \cdot (t/\degree C) + 6.94998 \times 10^{-5} \cdot (t/\degree C)^2 + 5.00002 \times 10^{-7} \cdot (t/\degree C)^3 \quad (1)
\]

\[
S/(\text{wt%}) = 9.0608 - 0.05911 \cdot (T/K) + 9.8925 \times 10^{-5} \cdot (T/K)^2 \quad (2)
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>10/°C</th>
<th>S/g·m⁻³</th>
<th>15/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2980</td>
<td>0</td>
<td>2971</td>
<td>0</td>
<td>2980</td>
</tr>
<tr>
<td>10</td>
<td>2630</td>
<td>10</td>
<td>2623</td>
<td>5</td>
<td>2760</td>
</tr>
<tr>
<td>20</td>
<td>2450</td>
<td>20</td>
<td>2444</td>
<td>20</td>
<td>2370</td>
</tr>
<tr>
<td>30</td>
<td>2470</td>
<td>25</td>
<td>2427</td>
<td>25</td>
<td>2340</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>2464</td>
<td>30</td>
<td>2360</td>
</tr>
</tbody>
</table>

**Rex 1906**

**Horvath 1982**

**Horvath & Getzen 1999**

**volumetric method**

**summary of literature data**

**tentative, IUPAC-NIST**

**temp range 273–303 K**

---

**FIGURE 5.1.2.6.1** Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for 1-bromopropane.

© 2006 by Taylor & Francis Group, LLC
TABLE 5.1.2.6.2
Reported vapor pressures of 1-bromopropane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + T/K) \quad (2) \\
\ln P &= A - B/(C + T/K) \quad (2a) \\
\log P &= A - B/(C + t/°C) \quad (3) \\
\ln P &= A - B/(C + t/°C) \quad (3a) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Rex 1906</th>
<th>Stull 1947</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>0</td>
<td>5546</td>
</tr>
<tr>
<td>10</td>
<td>9091</td>
</tr>
<tr>
<td>20</td>
<td>14772</td>
</tr>
<tr>
<td>30</td>
<td>22745</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1-bromopropane.
5.1.2.7 2-Bromopropane

\[ \text{Br} \]

Common Name: 2-Bromopropane
Synonym: isopropyl bromide
Chemical Name: 2-bromopropane, isopropyl bromide
CAS Registry No: 75-26-3
Molecular Formula: C\(_3\)H\(_7\)Br, CH\(_3\)CHBrCH\(_3\)
Molecular Weight: 122.992
Melting Point (°C):
   –89.0 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
   59.50 (Dean 1985; Lide 2003)
Density (g/cm\(^3\) at 20°C):
   1.3140, 1.3060 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
   93.6 (20°C, Stephenson & Malanowski 1987)
   97.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
   30.16, 28.4 (25°C, 58.6°C, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
   4180, 3650, 3180, 3180 (0, 10, 20, 30°C, volumetric method, Rex 1906)
   2877 (shake flask-volumetric method, Fühner 1924)
   3198 (30°C, shake flask, Van Arkel & Vles 1936)
   3162 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
   2880, 2690 (20°C, Korenman et al. 1971)
   3000 (selected exptl., Horvath 1982)
   2900 (18°C, Dean 1985)
   2860 (18°C, selected, Riddick et al. 1986)
   4160, 3640, 3170, 3170 (0, 10, 20, 30°C, tentative values of IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   23380, 35220 (20°C, 30°C, volumetric method Rex 1906)
   26664 (23.8°C, summary of literature data, temp range –61.8 to 60°C, Stull 1947)
   31500 (calculated by formula, Dreisbach 1961)
\[
\log (P/\text{mmHg}) = 6.61405 – 1072.9/(228.0 + t)\]°C; temp range –19 to 95°C (Antoine eq. for liquid state, Dreisbach 1955)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 7591.7/(T/K)] + 7.887729; \text{ temp range –61.8 to 60°C (Antoine eq., Weast 1972–73)}
\]
   28780 (interpolated-Antoine eq., Boublik et al. 1984)
\[
\log (P/\text{mmHg}) = 6.09819 – 1200.652/(233.815 + t\text{°C}); \text{ temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)}
\]
   31500 (selected, Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = 5.92741 – 1106.82/(222.851 + t\text{°C}); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]
   31940 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\[
\log (\text{P}_l/\text{mmHg}) = 5.28473 – 858.03/(–71.18 + T/K); \text{ temp range 236–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (\text{P}_l/\text{mmHg}) = 5.91155 – 1098.573/(–51.268 + T/K); \text{ temp range 299–332 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

© 2006 by Taylor & Francis Group, LLC
Halogenated Aliphatic Hydrocarbons

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 31.3032 - 2.4924 \times 10^3 \left( \frac{T}{\text{K}} \right) - 8.4645 \log \left( \frac{T}{\text{K}} \right) + 1.6459 \times 10^{-6} \left( \frac{T}{\text{K}} \right)^2; \]

temp range 184–532 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

1107 (calculated-1/K_w, C_w/C_A, reported as exp., Hine & Mookerjee 1975)
2479, 1564 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1082 (calculated-QSAR, Nirmalakhandan & Speece 1988)
978 (computed value, Yaws et al. 1991)
1192 (\( \gamma^\infty \) from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, \( \log K_{ow} \):

1.90 (calculated-\( \pi \) const., Hansch et al. 1968)
2.14 (recommended, Hansch et al. 1995)
1.80 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: \( k = 3.86 \times 10^{-6} \) s\(^{-1} \) with estimated \( t_{1/2} \sim 2.0 \) d at pH 7 and 25°C (Mabey & Mill 1978)
\( k = 1.4 \times 10^{-2} \) h\(^{-1} \) at pH 7 and 25°C with estimated \( t_{1/2} \sim 2.0 \) d (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986);
rate constants at 25°C: \( k = (379 \pm 41) \times 10^{-8} \) s\(^{-1} \) in distilled water at pH 3–11 for equal or more than 72% conversion (Mill et al. 1980; quoted, Haag & Mill 1988),
\( k = (383 \pm 33) \times 10^{-8} \) s\(^{-1} \) in distilled water for 89% conversion, \( k = (372 \pm 64) \times 10^{-8} \) s\(^{-1} \) in sediment-extracted water for 87% conversion, and \( k = (420 \pm 80) \times 10^{-8} \) s\(^{-1} \) in sediment pores at pH 7.3 for 88% conversion (Haag & Mill 1988).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance \( t_{1/2} \sim 2.4–24 \) h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water: estimated \( t_{1/2} \sim 2.0 \) d at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)
Ground water:
Sediment: \( t_{1/2} = 2.1 \) d, based on neutral and base-catalyzed hydrolysis studies at 25°C in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil:
Biota:
5.1.2.8 1,2-Dibromopropane

![Chemical Structure]

Common Name: 1,2-Dibromopropane
Synonym: propylene bromide, propylene dibromide
Chemical Name: 1,2-dibromopropane
CAS Registry No: 78-75-1
Molecular Formula:C₃H₆Br₂, CH₃CHBrCH₂Br
Molecular Weight: 201.888
Melting Point (°C):
  -55.49 (Lide 2003)
Boiling Point (°C):
  141.0 (Lide 2003)
Density (g/cm³ at 20°C):
  1.93268, 1.92344 (20°C, 25°C, Dreisbach 1959)
  1.9324, 1.9241 (20°C, 25°C, Dreisbach 1961)
  1.9324 (Horvath 1982; Weast 1982–83)
Molar Volume (cm³/mol):
  104.5 (20°C, calculated-density)
  120.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  42.43, 35.52 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  8.937 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  1430 (measured by Dow Chemical, Dreisbach 1955–1961)
  1463 (Hine & Mookerjee 1975)
  1428 (recommended, Horvath 1982)
  2000 (Dean 1985)
  2986 (calculated-fragment const., Wakita et al. 1986)
  1919 (predicted-MCI π and polarizability, Nirmalakhandan & Speece 1988)
  1420 (calculated-AI, Okouchi et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  2000 (37.3°C, Kahlbaum & Arndt 1898)
  1036 (Antoine eq. regression, temp range –7.0 to 141.6°C, Stull 1947)
  1071 (calculated-Antoine eq., Dreisbach 1959)
  log (P/mmHg) = 6.89105 – 1419.6/(212.0 + t⁰C); temp range 50–210°C (Antoine eq. for liquid state, Dreisbach 1959)
  688 (calculated by formula, Dreisbach 1961)
  log (P/mmHg) = 7.34875 – 1572.7/(212.0 + t⁰C); temp range 56–183°C (Antoine eq. for liquid state, Dreisbach 1961)
  log (P/mmHg) = [–0.2185 × 9801.9/(T/K)] + 8.073203; temp range –7.0 to 141.6°C (Antoine eq., Weast 1972–73)
  log (P/mmHg) = 7.30398 – 1644.4/(232.0 + t⁰C); temp range 0–50°C (Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 6.89105 – 1419.6/(212.0 + t⁰C); temp range 50–250°C (Antoine eq., Dean 1985, 1992)
  1072 (quoted from Dreisbach 1959, 1961, Riddick et al. 1986)
  log (P/kPa) = 6.01595 – 1419.6/(212.0 + t⁰C); temp range not specified (Antoine eq., Riddick et al. 1986)
  log (P/kPa) = 6.47365 – 1572.7/(–61.15 + T/K); temp range 329–456 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \( (P/L)/kPa) = 6.00898 - 1409.6/(62.856 + T/K) \); temp range 312–403 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 94.2 (calculated-\(1/K_{AW}, C_W/C_A\), reported as exptl., Hine & Mookerjee 1975)
- 21.1, 164 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 226.1 (calculated-QSAR, Nirmalakhandan & Speece 1988)
- 150 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \( log K_{OW} \):
- 2.54 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, \( log BCF \):

Sorption Partition Coefficient, \( log K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Hydrolysis: rate constant \( k = (2.5 \pm 0.5) \times 10^{-8} \text{ s}^{-1} \) in water at 25°C and pH 7 with \( t_{1/2} \approx 320 \text{ d} \) (Vogel & Reinhard 1986).

Half-Lives in the Environment:
- Air: disappearance \( t_{1/2} \approx 2.4–24 \text{ h} \) from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
5.1.2.9 1-Bromobutane (n-Butyl bromide)

Common Name: 1-Bromobutane
Synonym: n-butyl bromide, monobromobutane
Chemical Name: 1-bromobutane, n-butyl bromide, monobromobutane
CAS Registry No: 109-65-9
Molecular Formula: C₄H₉Br, CH₃CH₂CH₂CH₂Br
Molecular Weight: 137.02
Melting Point (°C): –112.6 (Lide 2003)
Boiling Point (°C):
  101.6 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  107.9 (20°C, calculated-density)
  119.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  36.60, 31.85 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  6.694 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  580 (16°C, volumetric method, Führner 1924)
  608 (30°C, shake flask-interferometer, Gross & Saylor 1931)
  598 (Seidell 1940; quoted, Deno & Berkerheimer 1960; Hine & Mookerjee 1975)
  254 (shake flask-volumetric method, Booth & Everson 1948)
  509 (exptl., Korenman et al. 1971)
  600 (selected exptl., Horvath 1982)
  869 (generator column-GC, Tewari et al. 1982)
  601 (calculated-UNIFAC activity coeff., Arbuckle 1986)
  608 (30°C, quoted, Riddick et al. 1986)
  680, 868, 871, 608 (16, 25, 25, 30°C, reported values, IUPAC-NIST Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  10972 (20°C, manometry, measured range 20–70°C, Smyth & Engel 1929)
  5333 (24.8°C, summary of literature data, measured range –33.0 to 101.6°C, Stull 1947)
  5502 (calculated by formula, Dreisbach 1961)
  log (P/mmHg) = 6.92254 – 1298.608/(219.70 + t/°C); temp range 19–141°C (Antoine eq. for liquid state, Dreisbach 1961)
  log (P/mmHg) = 6.92254 – 1298.608/(219.70 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
  log (P/mmHg) = [–0.2185 × 8789.1/(T/K)] + 8.028836; temp range –33.0 to 101.6°C (Antoine eq., Weast 1972–73)
  5502 (selected, Riddick et al. 1986)
  log (P/kPa) = 6.04744 – 1298.608/(219.70 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
  5502 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.04744 – 1298.608/(–53.45 + T/K); temp range 273–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \( (P/L/kPa) = 6.1388 - 1349.142/(–48.003 + T/K) \); temp range 338–373 K (Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log (P/mmHg) = 74.7061 - 4.0663 \times 10^3/(T/K) - 25.61 \cdot \log (T/K) + 1.3166 \times 10^{-2} \cdot (T/K)^2; \]
\[ \text{temp range 161–577 K (vapor pressure eq., Yaws 1994)} \]

\[ \ln (P/kPa) = 14.12331 - 3088.751/[(T/K) - 49.418]; \text{temp range 278.15–323.15 K (static method, Garriga et al. 2002)} \]

Henry's Law Constant (Pa m³/mol at 25°C):

1242 (calculated-\( I/K_{AX} \), \( C_W/C_A \), reported as exptl., Hine & Mookerjee 1975)
1600, 2313 (calculated-group contribution method, calculated-bond contribution Hine & Mookerjee 1975)
964.4 (calculated-QSAR, Nirmalakhandan & Speece 1988)
1223 (computed value, Yaws et al. 1991)
1215 (\( \gamma \) from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

2.75 (generator column-HPLC, DeVoe et al. 1981)
2.79 (estimated-activity coefficients, Wasik et al. 1981)
2.64 (estimated-activity coefficients, Schantz & Martire 1987)
2.75 (recommended, Sangster 1989)
2.75 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{1/2} \):

Half-Lives in the Environment:

Air: disappearance \( t_\text{1/2} = 2.4–24 \text{ h} \) for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976).
### 1-Bromopentane (n-Amyl bromide)

**Common Name:** 1-Bromopentane  
**Synonym:** n-amy1 bromide, monobromopentane, pentyl bromide  
**Chemical Name:** n-amy1 bromide, 1-bromopentane, monobromopentane, pentyl bromide  
**CAS Registry No:** 110-53-2  
**Molecular Formula:** C₅H₁₁Br, CH₃CH₂CH₂CH₂CH₂Br  
**Molecular Weight:** 151.045  
**Melting Point (°C):**  
-88.0 (Lide 2003)  
**Boiling Point (°C):**  
129.8 (Lide 2003)  
**Density (g/cm³ at 20°C):**  
1.2182, 1.2119 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)  
**Molar Volume (cm³/mol):**  
124.0 (20°C, calculated-density; Stephenson & Malanowski 1987)  
141.7 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, Δℍᵥ (kJ/mol):**  
41.78, 34.49 (25°C, at normal bp, Dreisbach 1961)  
41.43, 34.49 (25°C, bp, Riddick et al. 1986)  
**Enthalpy of Fusion, Δℍ₉₉ (kJ/mol):**  
11.46 (Riddick et al. 1986)  
**Entropy of Fusion, ΔS₉₉ (J/mol K):**  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m³ or mg/L at 25°C):**  
127 (generator column-GC, Tewari et al. 1982)  
141 (calculated-UNIFAC activity coeff., Arbuckle 1986)  
127 (selected, Riddick et al. 1986)  
127 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
1754 (calculated by formula, Dreisbach 1961)  
log (P/mmHg) = 6.95580 – 1401.634/(214.38 + t°C); temp range 41–171°C (Antoine eq. for liquid state, Dreisbach 1961)  
log (P/mmHg) = 6.95580 – 1401.634/(214.38 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)  
1680 (quoted, Riddick et al. 1986)  
log (P/kPa) = 6.08070 – 11401.634/(214.38 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)  
1680 (interpolated-Antoine eq., Malanowski 1987)  
log (P/kPa) = 6.0807 – 1401.634/(-58.77 + T/K); temp range 293–443 K (Antoine eq., Stephenson & Malanowski 1987)  
**Henry’s Law Constant (Pa m³/mol at 25°C):**  
2005 (computed value, Yaws et al. 1991)  
**Octanol/Water Partition Coefficient, log Kₒw:**  
3.37 (generator column-GC, DeVoe et al. 1981; Tewari et al. 1982)  
3.37 (generator column-HPLC, DeVoe et al. 1981)  
3.49 (generator column-GC, Wasik et al. 1981)  
3.32 (estimated-measured activity coefficients, Schantz & Martire 1987)  
3.37 (recommended, Sangster 1989)  
3.37 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
3.37 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

Air: disappearance $t_\text{½} = 2.4–24$ h for the reaction with OH radicals in air (USEPA 1974; quoted, Darnall et al. 1976).
### 5.1.2.11 1-Bromohexane

- **Common Name:** 1-Bromohexane
- **Synonym:** n-hexyl bromide
- **Chemical Name:** 1-bromohexane
- **CAS Registry No:** 111-25-1
- **Molecular Formula:** C₆H₁₃Br; CH₃(CH₂)₄CH₂Br
- **Molecular Weight:** 165.071
- **Melting Point (°C):** –83.7 (Lide 2003)
- **Boiling Point (°C):** 155.3 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
- **Density (g/cm³):**
  - 1.1744, 1.1667 (20°C, 25°C, Dreisbach 1961)
  - 1.1744 (20°C, Weast 1982–83)
- **Molar Volume (cm³/mol):**
  - 140.6 (20°C, calculated-density, Stephenson & Malanowski 1987)
  - 163.9 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Vaporization, ΔHV (kJ/mol):**
  - 46.77, 37.07 (25°C, bp, Dreisbach 1961)
- **Enthalpy of Fusion, ΔH_fus (kJ/mol):**
- **Entropy of Fusion, ΔS_fus (J/mol K):**
- **Fugacity Ratio at 25°C, F:** 1.0
- **Water Solubility (g/m³ or mg/L at 25°C):**
  - 25.75 (generator column-GC/FID, Tewari et al. 1982)
  - 25.8 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)
- **Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
  - 520 (calculated-Antoine eq., Dreisbach 1961)
  - log (P/mmHg) = 7.0023 – 1503.52/(209.5 + t°C); temp range 63–202°C (Antoine eq. for liquid state, Dreisbach 1961)
  - log (P/mmHg) = 7.0023 – 1503.52/(209.5 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
  - log (P/kPa) = 6.1272 – 1503.52/(T/K – 63.65); temp range 333–456 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)
- **Henry’s Law Constant (Pa·m³/mol):**
- **Octanol/Water Partition Coefficient, log K_{OW}:**
  - 3.80 (generator column-GC, Tewari et al. 1982)
  - 4.58 (HPLC-RT correlation, Burkhard et al. 1985)
  - 3.80; 3.804 (generator column-GC; calculated-activity coeff. γ, Schantz & Martire 1987)
  - 3.80 (recommended, Sangster 1989, 1993; Hansch et al. 1995)
- **Octanol/Air Partition Coefficient, log K_{OA}:**
- **Bioconcentration Factor, log BCF or log K_{B}:**
- **Sorption Partition Coefficient, log K_{OC}:**
- **Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:**

Half-Lives in the Environment:
5.1.2.12 1-Bromoheptane

Common Name: 1-Bromoheptane
Synonym: heptyl bromide
Chemical Name: 1-bromoheptane
CAS Registry No: 629-04-9
Molecular Formula: C\textsubscript{7}H\textsubscript{15}Br
Molecular Weight: 179.098

Melting Point (°C):
-56.1 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point (°C):
178.9 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Density (g/cm\textsuperscript{3}):
- 1.140, 1.1347 (20°C, 25°C, Dreisbach 1961)
- 1.140 (20°C, Weast 1982–83)

Molar Volume (cm\textsuperscript{3}/mol):
- 157.1 (20°C, calculated-density, Stephenson & Malanowski 1987)
- 186.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 51.83, 39.59 (25°C, bp, Dreisbach 1961)

Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 6.68 (generator column-GC/GID, Tewari et al. 1982; Miller et al. 1985)
- 6.68 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 163 (calculated-Antoine eq., Dreisbach 1961)
  \[
  \log (P/\text{mmHg}) = 7.0582 - 1603.71/(205.0 + t/°C); \text{ temp range } 82–228°C \ (\text{Antoine eq. for liquid state, Dreisbach 1961})
  \]
  \[
  \log (P/\text{mmHg}) = 7.0582 - 1603.71/(205.0 + t/°C); \text{ pressure range } 10 \text{ to } 1500 \text{ mmHg} \ (\text{Antoine eq. from correlation of selected lit. data, Li & Rossini 1961})
  \]
  \[
  \log (P/\text{mmHg}) = 6.1831 - 1603.71/(T/K – 68.15); \text{ temp range } 333–483 \text{ K} \ (\text{Antoine eq., liquid phase, Stephenson & Malanowski 1987})
  \]
  \[
  \log (P/\text{mmHg}) = 43.3327 - 4.0389 \times 10^{3}/(T/K) – 12.105 \log (T/K) – 1.5959 \times 10^{-10} \times (T/K)^{2}; \text{ temp range } 217–651 \text{ K} \ (\text{vapor pressure eq., Yaws 1994})
  \]

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 4.36 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
- 4.36; 4.44 (generator column-GC; calculated-activity coeff., Schantz & Mairtire 1987)
- 4.36 (recommended, Sangster 1989; 1994; Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
5.1.2.13 1-Bromooctane

Common Name: 1-Bromooctane
Synonym: octyl bromide
Chemical Name: 1-bromooctane
CAS Registry No: 111-83-1
Molecular Formula: C₈H₁₇Br, CH₃(CH₂)₆CH₂Br
Molecular Weight: 193.125

Melting Point (°C):
-55 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
200.8 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Density (g/cm³):
1.1122, 1.1072 (20°C, 25°C, Dreisbach 1961)
1.1122 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
174.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
208.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
56.92, 42.04 (25°C, bp, Dreisbach 1961)

Entropy of Fusion, ΔSₘₚ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1.67 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)
1.67 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)
1.72* (24.9°C, generator column-GC, measured range 1.1–40.1°C, Sarraute et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
50.66 (calculated-Antoine eq., Dreisbach 1961)
log (P/mmHg) = 7.1179 – 1701.61/(200.8 + t°C); temp range 101–253°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 7.1179 – 1701.61/(200.8 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
log (P₅/kPa) = 6.2428 – 1701.61/(T/K – 72.35); temp range 373–475 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
50.53* (24.9°C, calculated-Antoine eq. of Li & Rossini 1961, temp range 1.1–40.1°C, Sarraute et al. 2004)

Henry’s Law Constant (Pa·m³/mol at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
5699* (calculated-P/C, temp range 1.1–40.1°C, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, log Kₐₒₜₜ:
4.89 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
4.89; 5.09 (generator column-GC; correlated-activity coeff., Schantz & Martire 1987)
4.89 (recommended, Sangster 1989, 1994; Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₒₐ:

Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_c$:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>Table 5.1.2.13.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-bromo-octane at various temperatures and the coefficients for the vapor pressure equations:</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\log P &= A - \frac{B}{T} & (1) \\
\ln P &= A - \frac{B}{T} & (1a) \\
\log P &= A - \frac{B}{C + t} & (2) \\
\ln P &= A - \frac{B}{C + t} & (2a) \\
\log P &= A - \frac{B}{C + T} & (3) \\
\log P &= A - \frac{B}{T} - C\log(T) & (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sarraute et al. 2004</td>
<td>generator column-GC</td>
<td>extrapolated -Antoine eq.#</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$P/$Pa</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>1.10</td>
<td>2.66</td>
<td>1.10</td>
</tr>
<tr>
<td>5.0</td>
<td>2.22</td>
<td>5.0</td>
</tr>
<tr>
<td>5.2</td>
<td>2.414</td>
<td>5.2</td>
</tr>
<tr>
<td>9.9</td>
<td>1.76</td>
<td>9.9</td>
</tr>
<tr>
<td>9.9</td>
<td>1.77</td>
<td>9.9</td>
</tr>
<tr>
<td>14.9</td>
<td>1.82</td>
<td>14.9</td>
</tr>
<tr>
<td>24.9</td>
<td>1.715</td>
<td>24.9</td>
</tr>
<tr>
<td>29.9</td>
<td>2.18</td>
<td>29.9</td>
</tr>
<tr>
<td>34.0</td>
<td>2.78</td>
<td>34.0</td>
</tr>
<tr>
<td>40.0</td>
<td>3.65</td>
<td>40.0</td>
</tr>
<tr>
<td>40.1</td>
<td>3.48</td>
<td>40.1</td>
</tr>
</tbody>
</table>

Antoine eq.  
#see ref. Li & Rossini 1961  
eq 2  
P/mmHg  
A 7.1231  
B 1369.20  
C 204.4  
pressure range 10–1500 torr mmHg
5.1.2.14 1-Bromodecane

Common Name: 1-Bromodecane
Synonym: decyl bromide
Chemical Name: 1-bromohexane
CAS Registry No: 112-29-8
Molecular Formula: C_{10}H_{21}Br, CH_{3}(CH_{2})_{8}CH_{2}Br
Molecular Weight: 221.178

Melting Point (°C):
-29.2 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
240.6 (Dreisbach 1961; Weast 1982–83; Riddick et al. 1986; Lide 2003)

Density (g/cm³):
1.0702, 1.0656 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
1.0702 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
206.7 (10°C, Stephenson & Malanowski 1987)
252.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆H_v (kJ/mol):
67.12, 46.66 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ∆H_fus (kJ/mol):

Entropy of Fusion, ∆S_fus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.33 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 7.2336 – 1888.67/(193.3 + t/°C); temp range 135–297°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 7.2336 – 1888.67/(193.3 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

5.0 (quoted value from Dreisbach 1961, Riddick et al. 1986)

log (P/kPa) = 6.3585 – 1888.67/(193.3 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 6.3585 – 1888.67/(T/K – 79.85); temp range 383–570 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:
6.43 (HPLC-RT correlation, McDuffie 1981)
6.35, 5.84 (HPLC-RT correlation; calculated-CLOGP, Burkhard et al. 1985)
6.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF or log K_{b}:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_½:

Half-Lives in the Environment:
5.1.2.15 1-Bromododecane

Common Name: 1-Bromododecane
Synonym: lauryl bromide
Chemical Name: 1-bromododecane
CAS Registry No: 143-15-7
Molecular Formula: C₁₂H₂₅Br, CH₃(CH₂)₁₀CH₂Br
Molecular Weight: 249.231

Melting Point (°C):
-9.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point (°C):
276 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³):
1.0399, 1.0355 (20°C, 25°C, Dreisbach 1961)
1.0399 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
240.1 (20°C, Stephenson & Malanowski 1987)
297.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
77.38, 50.91 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔHᵥₙ (kJ/mol):

Entropy of Fusion, ΔSᵥₙ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

log (P/mmHg) = 7.3390 – 2061.93/(186.6 + t°C); temp range 165–237°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 7.3390 – 2061.93/(186.6 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini. 1961)

log (P/kPa) = 6.4639 – 2061.93/(T/K – 86.55); temp range 411–610 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_OW:
6.98; 6.90 (HPLC-RT correlation; calculated-CLOPG, Burkhard et al. 1985)

Octanol/Air Partition Coefficient, log K_OA:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_OC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Half-Lives in the Environment:
5.1.2.16 Bromocyclohexane

Common Name: Bromocyclohexane
Synonym: cyclohexyl bromide
Chemical Name: bromocyclohexane
CAS Registry No: 108-85-0
Molecular Formula: C₆H₁₁Br
Molecular Weight: 163.055
Melting Point (°C):
  –56.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  166.2 (Weast 1982–83; Lide 2003)
Density (g/cm³):
  1.33585, 1.32976 (20°C, 25°C, Dreisbach 1955)
  1.3359 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
  122.06, 122.6 (20°C, 25°C, calculated-density)
  141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  37.59, 44.80 (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  8.70 (Dreisbach 1955)
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  421 (calculated by formula, Dreisbach 1955)
  log (P/mmHg) = 6.97980 – 1572.19/(217.38 + t/°C); temp range 68–260°C (Antoine eq. for liquid state, Dreisbach 1955)
  log P/mmHg = 6.97980 – 1572.19/(t/°C + 217.38); temp range 68–200°C (Antoine eq., Dean 1992)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
  3.20 (shake flask-GC, Canton & Wagman 1983)
  3.20 (recommended, Sangster 1993)
  3.20 (selected, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log KOA:
Bioconcentration Factor, log BCF or log Kbi:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
5.1.2.17 Vinyl bromide

Common Name: Vinyl bromide
Synonym: bromoethene, bromoethylene, ethylene bromide
Chemical Name: bromoethene
CAS Registry No: 593-60-2
Molecular Formula: C\textsubscript{2}H\textsubscript{3}Br, CH\textsubscript{2} = CHBr
Molecular Weight: 106.949
Melting Point (°C):
-139.54 (Dreisbach 1959; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
15.80 (Dreisbach 1959; Dean 1985; Riddick et al. 1986; Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
1.4933, 1.4738 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
1.4930 (Dean 1985)
Molar Volume (cm\textsuperscript{3}/mol):
71.6 (20°C, calculated-density)
67.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
22.60, 23.45 (25°C, bp, Dreisbach 1959; Riddick et al. 1986)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
5.121 (Dreisbach 1959; Riddick et al. 1986)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
4310 (30°C, shake flask-interferometry, Saylor & Gross 1931)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
101325 (15.8°C, summary of literature data, temp range –95.4–15.8°C, Stull 1947)
137700 (calculated-Antoine eq., Dreisbach 1959) log (P/mmHg) = 6.66715 – 953.4/(236.0 + t°C); temp range –60 to 60°C (Antoine eq. for liquid state, Dreisbach 1959)
145350 (extrapolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 6076.9/(T/K)] + 7.490979; temp range –95.4 to 15.8°C (Antoine eq., Weast 1972–73)
144330, 139840 (calculated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 7.03256 – 1494.17/(281.722 + t°C); temp range –66–11.9°C (Antoine eq. derived from expdt data of Mehl 1934, Boublík et al. 1984)
log (P/kPa) = 6.08611 – 1083.017/(249.845 + t°C); temp range –87.5–16.0°C (Antoine eq. derived from expdt data of Guyer et al. 1937, Boublík et al. 1984)
137700 (selected lit. value, Riddick et al. 1986)
log (P/kPa) = 5.79205 – 953.4/(236.0 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
140480 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.03266 – 1014.0/(-37.15 + T/K); temp range 224–319 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –10.9281 – 1.1619 × 10\textsuperscript{3}/(T/K) + 9.3115 × 10\textsuperscript{-2}/(T/K) – 2.2655 × 10\textsuperscript{-2}/(T/K) – 4.531 × 10\textsuperscript{-5}/(T/K)\textsuperscript{2}; temp range 135–473 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 1.57 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
- 1.57 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO₃ radical and $k_{O_3}$ with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 6.81 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 25.4°C (Perry et al. 1977)
$k_{OH}(calc) = 6.6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(obs.) = 6.81 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672–4320$ h, based on aqueous screening test data for vinyl chloride (Hefgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2880–17280$ h, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24–2.4$ h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);
- $t_{1/2} = 9.4–94$ h, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344–69000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation of vinyl chloride from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
5.1.3 IODOALKANES

5.1.3.1 Iodomethane (Methyl iodide)

\[
\begin{align*}
\text{H} & \quad \text{I} \\
\text{H} & \\
\text{H}
\end{align*}
\]

Common Name: Methyl iodide
Synonym: iodomethane, moniodomethane
Chemical Name: methyl iodide
CAS Registry No: 74-88-4
Molecular Formula: CH$_3$I
Molecular Weight: 141.949
Melting Point (°C): –66.4 (Lide 2003)
Boiling Point (°C): 42.43 (Lide 2003)
Density (g/cm$^3$ at 20°C):
Molar Volume (cm$^3$/mol):
- 62.28 (20°C, calculated-density)
- 62.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 27.97, 27.338 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 14190* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
- 13630 (20°C, Merckel 1937)
- 14200 (Seidell 1940; Seidell 1941)
log $[C/(mol/L)] = –110.278 + 37.621 \cdot \log (T/K) + 4823/(T/K); \text{temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)}$
- 13900* (recommended, temp range 0–40°C, Horvath 1982)
- 14000 (20°C, Verschueren 1983; Riddick et al. 1986)
- 14000 (Dean 1985)

Vapor Pressure (Pa at 25°C, or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 44180, 64440(20°C, 30°C, Rex 1906)
- 75860* (34.4°C, temp range 0.10–34.4°C, Thompson & Linnett 1936)
- 53329* (25.3°C, summary of literature data, temp range –55.0 to 25.3°C, Stull 1947)
log $(P/mmHg) = 22.974 – 5.346 \cdot \log (T/K) – 2132/(T/K); \text{temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)}$
- 54120 (calculated-Antoine eq., Dreisbach 1961)
log $(P/mmHg) = 6.87991 – 1093.235/(230.94 + t°C); \text{temp range –29 to 76°C (Antoine eq. for liquid state, Dreisbach 1961)}$
log $(P/mmHg) = 6.87991 – 1093.235/(230.94 + t°C); \text{pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)}$
- 47750 (interpolated-Antoine eq., Weast 1972–73)
\[
\log (P/\text{mmHg}) = \left[ -0.2185 \times 6616.5/(T/\text{K}) \right] + 7.403018; \text{ temp range } -55.0 \text{ to } 254.8^\circ\text{C} \text{ (Antoine eq., Weast 1972–73)}
\]

53980 (calculated-Antoine eq., Kudchadker et al. 1979)

\[
\log (P/\text{mmHg}) = 6.97241 – 1138.29/(t/\text{°C} + 235.774); \text{ temp range } -14 \text{ to } 42^\circ\text{C} \text{ (Antoine eq., Kudchadker et al. 1979)}
\]

54120 (lit. average, Riddick et al. 1986)

\[
\log (P/\text{kPa}) = 6.09731 – 1138.29/(t/\text{°C} + 235.774); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

53960 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

\[
\log (P_{L}/\text{kPa}) = 6.10541 – 1142.67/(–36.87 + T/\text{K}); \text{ temp range } 228–337 \text{ K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

54009 (selected summary of literature data, temp range 206.71–363.15 K, Xiang 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

541*, 536 (exptl.-conc ratio, measured range 0–49°C, calculated-P/C, Glew & Moelwyn-Hughes 1953)

\[
\log \left( \frac{H}{(\text{mmHg} \cdot \text{L/mol})} \right) = 133.252 – 42.967 \cdot \log (T/\text{K}) – 6955.2/(T/\text{K}); \text{ temp range } 273.16–322.91 \text{ K (Glew & Moelwyn-Hughes 1953)}
\]

653* (29.43°C, concn ratio, measured range 29.43–40.34°C, Swain & Thornton 1962)

554.9 (calculated-I/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)

\[
\ln K_{AW} = 10.34 – 3541/(T/\text{K}); \text{ measured range } 5–33^\circ\text{C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)}
\]

287 (computed value, Yaws et al. 1991)

159, 442 (0, 20°C, distilled water, headspace-GC, Elliott & Rowland 1993)

429 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

414 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

\[
\log K_{AW} = 4.059 – 1416/(T/\text{K}) \text{ (summary of literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, log K_{OW}:

1.69 (19°C, shake flask, Collander 1951)

1.51 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

1.51 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.16 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: photooxidation t_{1/2} = 535–5348 h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Hydrolysis: k = 7.28 \times 10^{-8} \text{ s}^{-1} \text{ at pH } 7 \text{ (extrapolated to } 25^\circ\text{C}) \text{ with } t_{1/2} = 110 \text{ d (Mabey & Mill 1978).}

Biodegradation: aqueous aerobic t_{1/2} = 1168–672 h, based on estimated aerobic half-life (Howard et al. 1991); aqueous anaerobic t_{1/2} = 672–2688 h, based on estimated aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:
Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_{1/2} = 535–5348$ h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 168–672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 336–1344$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168–672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 5.1.3.1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reported aqueous solubilities of iodomethane (methyl iodide) at various temperatures</strong></td>
</tr>
<tr>
<td>$S/(wt%) = 1.53863 - 0.012169 \cdot (t/°C) + 1.2714 \times 10^{-4} \cdot (t/°C)^2 + 4.834 \times 10^{-6} \cdot (t/°C)^3$ (1)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Rex 1906</th>
<th>Horvath 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td>volumetric method</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g\cdot m^{-3}$</td>
</tr>
<tr>
<td>0</td>
<td>15650</td>
</tr>
<tr>
<td>10</td>
<td>14460</td>
</tr>
<tr>
<td>20</td>
<td>14190</td>
</tr>
<tr>
<td>30</td>
<td>14290</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 5.1.3.1.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for iodomethane.
TABLE 5.1.3.1.2
Reported vapor pressures of iodomethane (methyl iodide) at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\log P &= A - \frac{B}{C + t/\degree C} \quad (2) \\
\log P &= A - \frac{B}{T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\end{align*}
\]

Summary of literature data

<table>
<thead>
<tr>
<th>Thompson &amp; Linnett 1936</th>
<th>Stull 1947</th>
<th>Boublík &amp; Aim 1972</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/\degree C )</td>
<td>( P/Pa )</td>
<td>( t/\degree C )</td>
</tr>
<tr>
<td>0.10</td>
<td>18932</td>
<td></td>
</tr>
<tr>
<td>4.30</td>
<td>22798</td>
<td>-55.5</td>
</tr>
<tr>
<td>11.70</td>
<td>31331</td>
<td>-45.8</td>
</tr>
<tr>
<td>34.4</td>
<td>75860</td>
<td>-24.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-16.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-7.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>42.4</td>
</tr>
<tr>
<td></td>
<td>mp/\degree C</td>
<td>-64.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>eq. 2</td>
<td>P/kPa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodomethane.
TABLE 5.1.3.1.3
Reported Henry's law constants of iodomethane (methyl iodide) at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \quad (1) \\
\ln (1/K_{AW}) &= A - B/(T/K) \quad (2) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \quad (3) \\
\ln H &= A - B/(T/K) \quad (4) \\
K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 \quad (5) \\
\log H &= A - B\cdot\log (T/K) - C/(T/K) \quad (6)
\end{align*}
\]

Glew & Moelwyn-Hughes 1953
Swain & Thornton 1962
Elliot & Rowland 1993

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>169.9</td>
<td>29.45</td>
<td>653</td>
<td>0</td>
<td>159</td>
</tr>
<tr>
<td>5.03</td>
<td>224.8</td>
<td>29.44</td>
<td>651</td>
<td>20</td>
<td>442</td>
</tr>
<tr>
<td>10.2</td>
<td>288.0</td>
<td>40.35</td>
<td>923</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15.12</td>
<td>364.0</td>
<td>40.34</td>
<td>913</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.94</td>
<td>450.6</td>
<td></td>
<td></td>
<td>45</td>
<td>536</td>
</tr>
<tr>
<td>24.92</td>
<td>541.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>34.92</td>
<td>630.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>39.86</td>
<td>738.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>44.87</td>
<td>850.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>49.75</td>
<td>1072</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25.0</td>
<td>536</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

eq 6 P/(mmHg·L/mol)
A 71.005
B 21.656
C 4043.9

FIGURE 5.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for iodomethane.
### 5.1.3.2 Iodoethane (Ethyl iodide)

- **Common Name:** Ethyl iodide
- **Synonym:** iodoethane
- **Chemical Name:** ethyl iodide, iodoethane,
- **CAS Registry No:** 75-03-6
- **Molecular Formula:** C₂H₅I, CH₃CH₂I
- **Molecular Weight:** 155.965
- **Melting Point (°C):** –111.1 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)
- **Boiling Point (°C):** 72.30 (Rex 1906; Dreisbach 1961; Horvath 1982; Riddick et al. 1986; Lide 2003)
- **Density (g/cm³ at 20°C):**
  - 1.9358, 1.9245 (20°C, 25°C, Dreisbach 1961)
  - 1.9357, 1.9244 (20°C, 25°C, Riddick et al. 1986)
- **Molar Volume (cm³/mol):**
  - 80.6 (20°C, calculated from density)
  - 85.1 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Vaporization, ΔHV (kJ/mol):**
  - 31.93, 29.77 (25°C, bp, Riddick et al. 1986)
- **Enthalpy of Fusion, ΔH₉₅ (kJ/mol):**
- **Entropy of Fusion, ΔS₉₅ (J/mol K):**
- **Fugacity Ratio at 25°C, F:** 1.0

### Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 4030* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
- 3910 (22.5°C, volumetric method, Fühner 1924)
- 4040 (30°C, shake flask-interferometry, Gross & Saylor 1931)
- 3915 (20°C, shake flask, Van Arkel & Vles 1936)
- 3918 (20°C, Merckel 1937)
- 3915 (22.5°C, Saracco & Spaccamela Marchetti 1958)
- 3920 (20°C, exp tl., Korenman et al. 1971)
- 4041* (summary of literature data temp range 0–30°C, Horvath 1982)
- 3880 (30°C, selected, Riddick et al. 1986)
- 4000* (tentative value, temp range 0–30°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

\[ S/(\text{wt%}) = 8.5757 - 5.5568 \times 10^{-2}(T/K) + 9.43918 \times 10^{-5}(T/K)^2, \text{ temp range 273–303 K} \]

### Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 14280, 22150 (20°C, 30°C, Rex 1906)
- 21678* (30°C, manometry, measured range 30–60°C, Smyth & Engel 1929)
- 14612* (20°C, temp range –19.36 to 20.4°C, Milazzo 1944)
- 13332* (18°C, summary of literature data, temp range –54.4 to 72.4°C, Stull 1947)
- 18160 (calculated-Antoine eq., Dreisbach 1961)

\[ \log (P/\text{mmHg}) = 6.83198 - 1175.709/(225.26 + t/°C); \text{ temp range –6 to 109°C, (Antoine eq. for liquid state, Dreisbach 1961)} \]

\[ \log (P/\text{mmHg}) = 6.83198 - 1175.709/(225.26 + t/°C); \text{ pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)} \]

\[ \log (P/\text{mmHg}) = [-0.2185 \times 6843.1/(T/K)] + 7.635277; \text{ temp range –74.3 to 229.5°C (Antoine eq., Weast 1972–73)} \]
Halogenated Aliphatic Hydrocarbons

log (P/kPa) = 7.12695 – 1823.148/(285.30 + t/°C); temp range –19.36 to 20.4°C (Antoine eq. derived from reported exptl. data, Boublík et al. 1984)

log (P/kPa) = 6.06765 – 1222.410/(228.368 + t/°C), temp range 30–60°C (Antoine eq. derived from reported experimental data, Boublík et al. 1984)

log (P/mmHg) = 6.959 – 1232.0/(229.0 + t/°C); temp range 30–60°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 5.95688 – 1175.709/(225.26 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

18430 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 5.95686 – 1175.709/(-47.89 + T/K); temp range 249–369 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 31.4422 – 2.5719 × 10^3/(T/K) – 8.4867·log (T/K) – 9.0736 × 10^-11· (T/K)^2 + 3.571 × 10^-6·(T/K)^2; temp range 162–561 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

732 (calculated-1/K_{AW}, CW/CA, reported as exptl., Hine & Mookerjee 1975)

840 (calculated-QSAR, Nirmalakhandan & Speece 1988)

545 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.00 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.00 (recommended, Sangster 1989, 1993)

2.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

2.59 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioccentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

Hydrolysis: rate constant k = 1.62 × 10^-7 s^-1 with t_1/2 = 49 d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance t_1/2 = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: t_1/2 = 49 d at 25°C and pH 7 (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:
TABLE 5.1.3.2.1
Reported aqueous solubilities of 1-iodoethane at various temperatures

\[
\begin{align*}
S/(\text{wt} \%) &= 0.4391 - 3.24498 \times 10^{-3}\cdot(t/\degree\text{C}) + 4.49991 \times 10^{-5}\cdot(t/\degree\text{C})^2 + 1.15001 \times 10^{-6}\cdot(t/\degree\text{C})^3 \\
S/(\text{wt} \%) &= 8.5757 - 5.5568 \times 10^{-2}\cdot(T/\text{K}) + 9.43918 \times 10^{-4}\cdot(T/\text{K})^2
\end{align*}
\]

Volumetric method

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4410</td>
<td>0</td>
<td>4391</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>4140</td>
<td>10</td>
<td>4123</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>4030</td>
<td>20</td>
<td>4014</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>4041</td>
<td>30</td>
<td>4133</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Summary of literature data

<table>
<thead>
<tr>
<th>eq. 1</th>
<th>S/wt%</th>
<th>eq. 2</th>
<th>S/wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>4050</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Tentative, IUPAC-NIST

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4400</td>
</tr>
<tr>
<td>5</td>
<td>4220</td>
</tr>
<tr>
<td>10</td>
<td>4090</td>
</tr>
<tr>
<td>15</td>
<td>4010</td>
</tr>
<tr>
<td>20</td>
<td>3980</td>
</tr>
<tr>
<td>25</td>
<td>4000</td>
</tr>
<tr>
<td>30</td>
<td>4050</td>
</tr>
</tbody>
</table>

Temp range 273–303 K

FIGURE 5.1.3.2.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for iodoethane.
TABLE 5.1.3.2.2
Reported vapor pressures of iodoethane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th></th>
<th>Smyth &amp; Engel 1929</th>
<th>Milazzo 1944</th>
<th>Stull 1947</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>Manometry</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>30.0</td>
<td>21678</td>
<td>–19.36</td>
<td>1867</td>
</tr>
<tr>
<td>40.0</td>
<td>32637</td>
<td>0.040</td>
<td>5533</td>
</tr>
<tr>
<td>50.0</td>
<td>47329</td>
<td>9.34</td>
<td>8666</td>
</tr>
<tr>
<td>60.0</td>
<td>67448</td>
<td>10.4</td>
<td>9066</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20.4</td>
<td>14612</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for iodoethane.
5.1.3.3 1-Iodopropane

Common Name: 1-Iodopropane
Synonym: moniodopropane, \( n \)-propyl iodide, propyl iodide
Chemical Name: 1-iodopropane, moniodopropane, \( n \)-propyl iodide, propyl iodide
CAS Registry No: 107-08-4
Molecular Formula: \( \text{C}_3\text{H}_7\text{I}, \text{CH}_3\text{CH}_2\text{CH}_2\text{I} \)
Molecular Weight: 169.992
Melting Point (°C):
-101.3 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
102.5 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
1.7489, 1.7394 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
97.2 (20°C, calculated-density)
107.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
45.98, 31.70 (25°C, bp, Dreisbach 1961)
36.25 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1070* (20°C, volumetric method, measured range 0–30°C, Rex 1906)
867 (20°C, volumetric method, Fühner 1924)
1040 (30°C, shake flask-interferometer, Gross & Saylor 1931)
1037 (30°C, shake flask, Van Arkel & Vles 1936)
1073 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)
872 (Seidell 1941)
1110 (calculated-\( K_{\text{ops}} \), Hansch et al. 1968)
1070, 1060 (23.5°C, elution chromatography, Schwarz 1980)
1051* (summary of literature data, temp range 0–30°C, Horvath 1982)
1000 (Dean 1985)
1040 (30°C, quoted, Riddick et al. 1986)
1010* (tentative value, temp range 0–30°C, IUPAC-NIST Series, Horvath & Getzen 1999b)
\[ S/(\text{wt}\%) = 3.4659 - 0.023046 \cdot (T/K) + 3.94424 \times 10^{-5} \cdot (T/K)^2 \] temp range 273–303 K (equation derived from literature data, Horvath & Getzen 1999b)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4679, 7305 (20°C, 30°C, volumetric method Rex, 1906)
5333 (23.6°C, summary of literature, data temp range –36.0 to 102.5°C, Stull 1947)
5745 (calculated-Antoine eq., Dreisbach 1961)
\[ \log (\text{P/mmHg}) = 6.81603 - 1267.062/(219.53 + t/°C) \] temp range 18–143°C (Antoine eq. for liquid state, Dreisbach 1961)
\[ \log (\text{P/mmHg}) = 6.81603 - 1267.062/(219.53 + t/°C) \] pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
\[ \log (\text{P/mmHg}) = [-0.2185 \times 8467.1/(T/K)] + 7.824521; \text{temp range } -36.0 \text{ to } 102.5°C \] (Antoine eq., Weast 1972–73)
5745 (quoted lit. average, Riddick et al. 1986)
\[ \log (\text{P/kPa}) = 5.94053 - 1267.062/(219.53 + t/°C) \] temp range not specified (Antoine eq., Riddick et al. 1986)
Halogenated Aliphatic Hydrocarbons

5745 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
\[ \log (P_t/kPa) = 5.6036 - 1160.5/(-59.55 + T/K); \text{ temp range 171–271 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]
\[ \log (P_t/kPa) = 5.94093 - 1267.062/(-52.62 + T/K); \text{ temp range 271–402 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]
\[ \log (P/mmHg) = 1.2733 - 2.0214 \times 10^{-3}/(T/K) + 4.1138 \cdot \log (T/K) - 1.2477 \times 10^{-2} \cdot (T/K) + 7.678 \times 10^{-6} \cdot (T/K)^2; \text{ temp range 172–593 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa m³/mol at 25°C):
921 (calculated as \(1/K_{AW} \cdot C_N/C_A\), reported as exptl., Hine & Mookerjee 1975)
1033, 1082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1057 (calculated-QSAR, Nirmalakhandan & Speece 1988)
844 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \(K_{ow}\):
2.50 (calculated-\(\pi\) const., Hansch et al. 1968)

Bioconcentration Factor, \(K_{bcf}\):

Sorption Partition Coefficient, \(K_{oc}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_1/2\):

Half-Lives in the Environment:
Air: disappearance \(t_{1/2} = 2.4–24\) h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

### TABLE 5.1.3.3.1
Reported aqueous solubilities of 1-iodopropane at various temperatures

\[
\begin{align*}
S/(wt\%) &= 0.1139 - 4.86669 \times 10^{-4} \cdot (T/°C) + 1.25003 \times 10^{-5} \cdot (T/°C)^2 - 2.8334 \times 10^{-3} \cdot (T/°C)^3 \quad (1) \\
S/(wt\%) &= 3.4659 - 0.023046 \cdot (T/K) + 3.94424 \times 10^{-5} \cdot (T/K)^2 \quad (2)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Rex 1906</th>
<th>Horvath 1982</th>
<th>Horvath &amp; Getzen 1999b</th>
</tr>
</thead>
<tbody>
<tr>
<td>volumetric method</td>
<td>summary of literature data</td>
<td>tentative, IUPAC-NIST</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
</tr>
<tr>
<td>0</td>
<td>1140</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>1030</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>1070</td>
<td>20</td>
</tr>
<tr>
<td>30</td>
<td>1030</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>1051</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1029</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>temp range 273–303 K</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
**FIGURE 5.1.3.3.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-iodopropane.
5.1.3.4 2-Iodopropane

Common Name: 2-Iodopropane
Synonym: isopropyl iodide
Chemical Name: 2-iodopropane, isopropyl iodide
CAS Registry No: 75-30-9
Molecular Formula: C₃H₇I, CH₃CHICH₃
Molecular Weight: 169.992
Melting Point (°C):
  −90.0 (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
  89.50 (Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 20°C):
  1.7042, 1.6946 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  99.8, 100.3 (20°C, 25°C, calculated-density)
  107.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  34.06 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  1670, 1430, 1400, 1340 (0, 10, 20, 30°C, volumetric method, Rex 1906)
  1343 (30°C, shake flask, Van Arkel & Vles 1936)
  1667, 1428, 1398, 1387, 1338 (0, 10, 20, 25, 30°C, summary of literature data, Horvath 1982)
  S/(wt%) = 0.1667 – 4.23167 × 10⁻³·u/°C + 0.000224·(u/°C)² – 3.98334 × 10⁻⁶·(u/°C)³ (Horvath 1982)
  1400 (20°C, selected, Riddick et al. 1986)
  1670, 1430, 1400, 1340 (0, 10, 20, 30°C, reported expxtl data of Rex 1906, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  7518, 11780 (20°C, 30°C, Rex 1906)
  7999 (21.6°C, summary of literature data, temp range −43.3 to 89.5°C, Stull 1947)
  log (P/mmHg) = [ −0.2185 × 8243.4/(T/K) ] + 7.873828; temp range −43.3 to 89.5°C (Antoine eq., Weast 1972–73)
  5700 (selected, Riddick et al. 1986)
  log (P/kPa) = 6.87492 – 1765.15/(T/K); temp range not specified (Antoine eq., Riddick et al. 1986)
  9360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  log (P/KPa) = 6.2763 – 1414.85/(−31.45 + T/K); temp range 261–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 5.2724 – 989.55/(−69.18 + T/K); temp range 173–262 K (Antoine eq.-II, Stephenson & Malanowski 1987)
  log (P/mmHg) = 33.2023 – 2.7569 × 10³/(T/K) – 9.0585 log (T/K) – 1.2099 × 10⁻¹⁰(T/K) + 3.5044 × 10⁻⁶(T/K)²; temp range 183–578 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
  1133 (calculated-1/KAW, CW/CAM, reported as expxtl., Hine & Mookerjee 1975)
  2479, 1982 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
  1840 (calculated-QSAR, Nirmalakhandan & Speece 1988)
  903 (computed value, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log $K_{OW}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant $k = 2.77 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 2.9 \text{ d}$ at $25^\circ\text{C}$ and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: $t_{1/2} = 2.9 \text{ d}$ at $25^\circ\text{C}$ and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:
5.1.3.5 1-Iodobutane

Common Name: 1-Iodobutane
Synonym: \( n \)-butyl iodide, monoiodobutane
Chemical Name: \( n \)-butyl iodide, 1-iodobutane, monoiodobutane
CAS Registry No: 542-69-8
Molecular Formula: \( \text{C}_4\text{H}_9\text{I} \), \( \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I} \)
Molecular Weight: 184.018

Melting Point (°C):
-103.0  (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):
130.53  (Dreisbach 1961; Riddick et al. 1986)
130.5   (Lide 2003)

Density (g/cm³ at 20°C):
1.6154, 1.6072  (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm³/mol):
113.9, 114.5 (20°C, 25°C, calculated-density, Riddick et al. 1986)
129.5    (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta \text{H}_v \) (kJ/mol):
40.63, 33.40 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta \text{H}_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta \text{S}_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
210    (17.5°C, volumetric method, Fühner 1924)
202    (20°C, Merckel 1937)
211    (Seidell 1940; quoted, Deno & Berkheimer 1960)
202    (Seidell 1941)
313    (Kakovskv 1957)
182    (selected exptl., Horvath 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1848   (calculated-Antoine eq., Dreisbach 1961)

\[ \log (P/\text{mmHg}) = 6.82262 - 1358.860/(214.2 + t/°C); \text{ temp range 40–174°C (Antoine eq. for liquid state, Dreisbach 1961)} \]

\[ \log (P/\text{mmHg}) = 6.82262 - 1358.860/(214.20 + t/°C); \text{ pressure range of 10 to 1500 mmHg (Antoine eq., from correlation of selected lit. data, Li & Rossini 1961)} \]

\[ \log (P/\text{kPa}) = 5.94752 - 1358.860/(214.20 + t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)} \]
1848   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P/\text{kPa}) = 5.94752 - 1358.860/(-58.95 + T/K); \text{ temp range 292–431 K (Antoine eq., Stephenson & Malanowski 1987)} \]

Henry’s Law Constant (Pa m³/mol at 25°C):
1600    (calculated-\( 1/K_{\text{AW}} \), \( C_w/C_A \), reported as exptl., Hine & Mookerjee 1975)
1426, 600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1331    (calculated-QSAR, Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
3.00    (calculated-\( \pi \) const., Hansch et al. 1968)
2.51    (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).
5.1.3.6 1-Iodopentane

Common Name: 1-Iodopentane
Synonym: pentyl iodide
Chemical Name: 1-iodopentane
CAS Registry No: 628-17-1
Molecular Formula: C₅H₁₁I, CH₃(CH₂)₃CH₂I
Molecular Weight: 198.045

Melting Point (°C):
-85.6 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
157 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³):
1.5061, 1.5088 (20°C, 25°C, Dreisbach 1961)
1.5161 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
130.6 (20°C, calculated-density, Stephenson & Malanowski 1987)
151.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
43.33, 35.81 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔHₚ (kJ/mol):

Entropy of Fusion, ΔSₚ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
585 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.85172 – 1454.028/(209.17 + t°C); temp range 61–204°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.85172 – 1454.028/(209.17 + t°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

log Pₗ/kPa = 5.97662 – 1454.028/(-63.98 + T/K); temp range 312–413 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kₐₜₜ:

Octanol/Air Partition Coefficient, log K₀ₐ:

Bioconcentration Factor, log BCF or log Kₘ:

Sorption Partition Coefficient, log Kₙ:

Environmental Fate Rate Constants, k, and Half-Lives, tᵢₚ:

Half-Lives in the Environment:
5.1.4 Mixed Halogenated Hydrocarbons

5.1.4.1 Bromochloromethane

Common Name: Bromochloromethane  
Synonym: chlorobromomethane, methylene bromochloride  
Chemical Name: bromochloromethane, chlorobromomethane  
CAS Registry No: 74-97-5  
Molecular Formula: CH₂BrCl  
Molecular Weight: 129.384  
Melting Point (°C): -87.9 (Lide 2003)  
Boiling Point (°C): 68.0 (Lide 2003)  
Density (g/cm³ at 20°C):  
1.9344 (Dreisbach 1959; Weast 1982–83; Riddick et al. 1986)  
1.9229 (25°C, Dreisbach 1959)  
Molar Volume (cm³/mol):  
66.89 (20°C, calculated-density)  
73.8 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):  
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
15000 (O’Connell 1963)  
9000 (Kirk-Othmer 1964, Irmann 1965, Dean 1985)  
15000 (Jolls 1966)  
14778 (at saturated pressure, recommended, Horvath 1982)  
16690 (generator column-GC, Tewari et al. 1982)  
38900 (calculated-UNIFAC activity coeff., Arbuckle 1986)  
17000 (selected, Riddick et al. 1986)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
18808 (24.06°C, ebulliometric method, measured range 15.72–68°C, McDonald et al. 1959)  
\[ \log (P/\text{mmHg}) = 6.38587 - 895.556/(186.703 + t/°C); \text{temp range 15.72–68.0°C (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)} \]  
19620 (calculated-Antoine eq., Dreisbach 1959)  
\[ \log (P/\text{mmHg}) = 6.86624 - 1132.3/(215.0 + t/°C); \text{temp range –6 to 297°C (Antoine eq. for liquid state, Dreisbach 1959)} \]  
19520 (calculated-Antoine eq., Boublik et al. 1973)  
\[ \log (P/\text{mmHg}) = 6.49606 - 942.267/(192.587 + t/°C); \text{temp range 15.7–68°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)} \]  
19520 (calculated-Antoine eq., Kudchadker et al. 1979)  
\[ \log (P/\text{mmHg}) = 6.41307 - 903.382/(187.594 + t/°C); \text{temp range 16–68°C (Antoine eq., Kudchadker et al. 1979)} \]  
\[ \log (P/\text{kPa}) = 6.60056 - 932.609/(191.376 + t/°C); \text{temp range 15.7–68°C (Antoine eq. from reported exptl. data of McDonald & Shrader 1959, Boublik et al. 1984)} \]  
19530 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
\[ \log (P_t/\text{kPa}) = 5.51146 - 891.345/(–86.965 + T/K); \text{temp range 226–341 K (Antoine eq., Stephenson & Malanowski 1987)} \]
log (P/mmHg) = 2.7704 – 2.0139 × 10^{3}/(T/K) + 3.7817·log (T/K) – 1.3241 × 10^{–2}·(T/K) + 8.1979 × 10^{–6}·(T/K)^2;  
19257 (selected summary of literature data, temp range 185.21–368.15 K, Xiang 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:

1.41 (generator column-GC, Tewari et al. 1982)
1.41 (recommended, Sangster 1993)
1.41 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:
Photolysis:
Oxidation:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:  
rate constant for the reaction with OH–: k = (2.5 ± 0.3) × 10^{–6} M^{-1} s^{-1} was measured in 66.7% dioxane-water  
at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)

k_{OH} = 1.11 × 10^{–13} cm^3 molecule^{-1} s^{-1} with atmospheric lifetime τ = 0.43 yr at 298 K, measured range  
277–377 K (flash photolysis resonance fluorescence and discharge flow electron paramagnetic resonance,  
Orkin et al. 1997)
Hydrolysis: rate constant k = 1.2 × 10^{–10} s^{-1} with t_{1/2} = 44 yr at pH 7 and 25°C (Mabey & Mill 1978)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance t_{1/2} = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et 
al. 1976)
Atmospheric lifetime τ = 0.21 yr reduced from 0.43 yr due to reaction with OH with ocean removal (Orkin et al.  
1997)
Surface water: hydrolysis rate constant k = 1.2 × 10^{–10} s^{-1} with t_{1/2} = 44 yr at pH 7 and 25°C (Mabey & Mill 1978)
5.1.4.2 Bromodichloromethane

\[
\begin{array}{c}
\text{Cl} \\
\text{Cl} \\
\text{H} \\
\text{Br}
\end{array}
\]

Common Name: Bromodichloromethane
Synonym: dichlorobromomethane
Chemical Name: bromodichloromethane, dichlorobromomethane
CAS Registry No: 75-27-4
Molecular Formula: 
Molecular Weight: 163.829
Melting Point (°C):
-57 (Lide 2003)
Boiling Point (°C):
90.0 (Weast 1977; Lide 2003)
Density (g/cm³ at 20°C):
1.9710 (25°C, Verschueren 1983)
Molar Volume (cm³/mol):
83.1 (20°C, calculated-density)
94.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
4700 (22°C, Mabey et al. 1981)
2968 (30°C, headspace-GC, McNally & Grob 1984)
8880, 8668, 8506 (20, 30, 40°C, infinite dilution activity coeff. \( \gamma \)-GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6665 (20°C, Dreisbach 1952;)
8555, 13440, 20444 (20, 30, 40°C, DIPPR compilation, Tse et al. 1992)

Henry’s Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations):
244.2 (20°C, calculated-P/C, Mabey et al. 1982)
162 (20°C, batch air stripping-GC, Nicholson et al. 1984)
162, 152, 152 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

ln \[ H/(\text{atm m}^3/\text{mol}) \] = 11.30 – 5210/(T/K); temp range 10–30°C (air stripping-GC measurements, Nicholson et al. 1984)
214.8 (gas stripping-GC, Warner et al. 1987)
243 (calculated-P/C, Mackay & Shiu 1990)
162, 263, 405 (20, 30, 40°C, infinite dilution activity coeff. \( \gamma \)-GC, Tse et al. 1992)
55.2, 106, 192 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

ln \( K_{\text{AW}} \) = 13.43 – 4678/(T/K); seawater of salinity of 30.4‰, temp range: 0–10°C (Moore et al. 1995)
185 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

\[ \log K_{\text{AW}} = 6.143 – 2130/(T/K) \] (summary of literature data, Staudinger & Roberts 2001)
347 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):
1.88 (calculated as per Tute 1971, Callahan et al. 1979; Mills et al. 1982)
2.10 (Hansch & Leo 1979)
2.10 (calculated, Mabey et al. 1982)
2.00 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$

$2.98; 2.97$ (equilibrium headspace-GC; calculated-$K_{OW}/K_{AW}$, Batterman et al. 2002)

Bioconcentration Factor, log BCF:

$1.544$ (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)

$0.72–1.37$ (estimated as per Lyman et al. 1982, Howard 1990)

Sorption Partition Coefficient, log $K_{OC}$:

$1.785$ (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)

$1.724–2.40$ (estimated from S & $K_{OW}$, Swann et al. 1983; quoted, Howard 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization: typical $t_{1/2} \approx 35$ h for a range of 33 min to 12 d was estimated from experimentally determined gas transfer rates (Kaczmar et al. 1984; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: calculated rate constants at 25°C. $k \ll 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 0.2$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: first-order rate constant $k = 1.6 \times 10^{-10}$ s$^{-1}$ at pH 7 and 25°C with a maximum $t_{1/2} = 137$ yr (Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard 1990).

Biodegradation:

Biotransformation: estimated rate constant $k = 1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4–24$ h from air for the reaction with OH radical (Darnall et al. 1976);

$3.92$ months, based on an estimated rate constant $k = 8.522 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the vapor phase reaction with hydroxyl radical (GEMS 1987; quoted, Howard 1990).

Surface water: hydrolysis rate constant $k = 1.6 \times 10^{-10}$ s$^{-1}$ with $t_{1/2} = 137$ yr at pH 7 and 25°C (Mabey & Mill 1978)
5.1.4.3 Dibromochloromethane

Common Name: Dibromochloromethane
Synonym: chlorodibromomethane
Chemical Name: dibromochloromethane, chlorodibromomethane
CAS Registry No: 124-48-1
Molecular Formula: CHBr₂Cl
Molecular Weight: 208.280

Melting Point (°C):
-22.0 (Dean 1985)
-20 (Lide 2003)

Boiling Point (°C):
119–120 (Weast 1977; Weast 1982–83)
120 (Lide 2003)

Density (g/cm³ at 20°C):
2.451 (Weast 1982–83; Dean 1985)

Molar Volume (cm³/mol):
84.98 (20°C, calculated-density)
97.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C):
4000 (calculated-K_w, Mabey et al. 1982)
5814, 6000, 6102 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
10131 (20°C, extrapolated-Antoine eq., Mabey et al. 1982)
2000 (20°C, selected, Mills et al. 1982)
6667 (20°C, Warner et al. 1987)
2324, 3877, 6232 (20, 30, 40°C, DIPPR compilation, Tse et al. 1992)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
100 (20°C, calculated-P/C, Mabey et al. 1982)
88.2; 88.1, 85.1 (20°C, batch air stripping-GC; quoted lit. values, Nicholson et al. 1984)
86.1, 81.06, 78.02 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
ln [H/(atm m³/mol)] = 10.70 – 5210/(T/K); temp range 10–30°C (air stripping-GC measurements, Nicholson et al. 1984)
80.4 (gas stripping-GC, Warner et al. 1987)
120* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m³/mol)] = 14.62 – 6373/(T/K); temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)
100 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
81.06, 142, 223 (20, 30, 40°C, infinite dilution activity coeff. γ-GC, Tse et al. 1992)
28.2, 56.3, 103 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
ln K_AW = 13.62 – 4914/(T/K); seawater of salinity of 30.4‰, temp range: 0–10°C (Moore et al. 1995)
85.3 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
log K_AW = 6.296 – 2273/(T/K) (summary of literature data, Staudinger & Roberts 2001)
218 (37°C, equilibrium headspace-GC, Batterman et al. 2002)
Halogenated Aliphatic Hydrocarbons

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 2.09 (calculated as per Tute 1971, Callahan et al. 1979)
- 2.24 (Hansch & Leo 1979)
- 2.24 (calculated, Mabey et al. 1982)
- 2.16 (recommended, Sangster 1993)
- 2.04 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C:
- 3.59 (calculated-measured infinite dilution activity coeff. and vapor pressure $P$, Abraham et al. 2001)
- 3.33; 3.31 (equilibrium headspace-GC; calculated-$K_{ow}/K_{aw}$, Batterman et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization: calculated $t_\frac{1}{2} = 43$ min to 16.6 d (using Langbein & Durum 1967 published O$_2$ re-aeration values) and $t_\frac{1}{2} = 45.9$ h both from rivers and streams (Kaczmar et al. 1984).
- Photolysis:
  - Oxidation: calculated rate constants at 25°C: $k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 0.5$ M$^{-1}$ h$^{-1}$ for peroxy radicals (Mabey et al. 1982);
  - photooxidation $t_\frac{1}{2} = 1025-10252$ h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- Hydrolysis: rate constant $k = 8.0 \times 10^{-11}$ s$^{-1}$ with hydrolytic $t_\frac{1}{2} = 274$ yr at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard et al. 1991);
  - $k = 2.88 \times 10^{-8}$ h$^{-1}$ at pH 7 and 25°C (analogy to chloroform as per Mabey & Mill 1978, Mabey et al. 1982).
- Biodegradation: aqueous aerobic $t_\frac{1}{2} = 672-4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_\frac{1}{2} = 672-4320$ h, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; Bouwer et al. 1981; quoted, Howard et al. 1991).
- Biotransformation: estimated rate constant $k = 1.0 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
- Air: disappearance $t_\frac{1}{2} = 2.4-24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_\frac{1}{2} = 1025-10252$ h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- Surface water: $t_\frac{1}{2} = 274$ yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)
  - $t_\frac{1}{2} = 672-4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).
- Ground water: $t_\frac{1}{2} = 336-4320$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).
- Sediment:
  - Soil: $t_\frac{1}{2} = 672-4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).
- Biota:
**TABLE 5.1.4.3.1**
Reported Henry’s law constants of dibromochloromethane at various temperatures

Ashworth et al. 1988

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>38.50</td>
</tr>
<tr>
<td>15</td>
<td>45.60</td>
</tr>
<tr>
<td>20</td>
<td>104.4</td>
</tr>
<tr>
<td>25</td>
<td>119.6</td>
</tr>
<tr>
<td>30</td>
<td>154.0</td>
</tr>
</tbody>
</table>

\[
\ln \left[ \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right] = A - \frac{B}{(T/\text{K})}
\]

A 14.62
B 6373

**FIGURE 5.1.4.3.1** Logarithm of Henry’s law constant versus reciprocal temperature for dibromochloromethane.
5.1.4.4 Chlorodifluoromethane (HCFC-22)

Common Name: Chlorodifluoromethane
Synonym: difluorochloromethane, Freon 22, CFC-22, CF-22
Chemical Name: chlorodifluoromethane
CAS Registry No: 75-45-6
Molecular Formula: CHClF₂
Molecular Weight: 86.469
Melting Point (°C):
  -157.42 (Lide 2003)
Boiling Point (°C):
  -40.7 (Lide 2003)
Density (g/cm³ at 20°C):
  1.2090 (21°C, Dean 1985)
  1.1940 (25°C, Kirk-Othmer 1985)
Molar Volume (cm³/mol):
  71.2 (20°C, calculated-density)
  60.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
  20.238 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆H₉ (kJ/mol):
  4.123 (Riddick et al. 1986)
Entropy of Fusion, ∆S₉ (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
  2800, 2900 (quoted values, Irmann 1965)
  3000 (DuPont 1966, 1969; quoted, Horvath 1982; Riddick et al. 1986)
  2930 (selected, Hine & Mookerjee 1975)
  3000 (Weast 1976; quoted, Horvath 1982)
  2899* (summary of literature data, temp range 0–60°C, Horvath 1982)
  3000 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  101325* (~40.8°C, summary of literature data, temp range –122.8 to –40.8°C, Stull 1947)
  1083100 (calculated-Antoine eq., Weast 1972–73)
  log (P/mmHg) = [–0.2185 × 5212.9/(T/K)] + 7.730042; temp range –122.8 to 85.3°C (Antoine eq., Weast 1972–73)
  log (P/mmHg) = 6.93892 – 808.919/(t°C + 240.161); temp range –79 to –37°C (Antoine eq., Kudchadker et al. 1979)
  1027400 (calculated-Antoine eq., Boublík et al. 1984)
  log (P/kPa) = 6.0741 – 815.920/(241.369 + t°C) (Antoine eq. from reported exptl. data, Boublík et al. 1984)
  35120, 570500 (~61.26°C, 4.5°C, Riddick et al. 1986)
  log (P/kPa) = 6.06382 – 808.919/(240.161 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
  1043900 (Interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.33292 – 919.834/(–19.718 + T/K); temp range 170–233 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \( \left( \frac{P}{kPa} \right) = 6.19138 - 863.436/(26.04 + T/K) \); temp range 230–275 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( \left( \frac{P}{kPa} \right) = 6.35713 - 950.38/(13.474 + T/K) \); temp range 275–327 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log \( \left( \frac{P}{kPa} \right) = 7.13064 - 1490.048/(64.627 + T/K) \); temp range 324–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

\[ \log (P/mmHg) = 40.3847 - 2.0731 \times 10^3/(T/K) - 12.317 \cdot \log (T/K) - 2.5116 \times 10^{-10} \cdot (T/K)^2; \]
temp range 116–369 K (vapor pressure eq., Yaws 1994)

132020 (238.15 K, selected summary of literature data, temp range 15.74–238.15 K, Xiang 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C):

log \( \left( \frac{H}{atm} \right) = 8.18 - 1469.55/(T/K) \) (least-square regression of data from lit., Kavanaugh & Trussell 1980)

2980 (calculated as \( 1/K_{AW}, C_W/C_A \), reported as expl., Hine & Mookerjee 1975)

2478.8 (calculated-QSAR, Nirmalakhandan & Speece 1988)

3058 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

1.08 (shake flask, Log P Database, Hansch & Leo 1987)

1.08 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3 (as indicated), data at other temperatures and/or the Arrhenius expression

\( k_{OH}^\circ = (4.75 \pm 0.48) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K, measured range 297–434 K, with estimated lifetime of \( \sim 1.5 \text{ yr} \) (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

\( k_{OH} = (3.4 \pm 0.7) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

\( k_{OH}^\circ = (4.25 \pm 0.28) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K, measured range 253–427 K, with calculated lifetime of 16–25 yr in troposphere (discharge flow-resonance fluorescence, Chang & Kaufman 1977)

\( k_{OH} = 4.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K with lifetime of 43 yr in troposphere, measured range 250–350 K (FP-RF, Watson et al. 1977; quoted, Altshuller 1980)

\( k_{OH} = (2.76 \pm 0.35) \times 10^9 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 297 K (relative rate, Paraskevopoulos et al. 1981)

\( k_{OH}^\circ = 6.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), and \( k_{OH}(\text{obs.}) = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (SAR [structure-activity relationship], Atkinson 1985)

\( k_{OH}^\circ = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1989)

\( k_{OH} = 4.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with an estimated tropospheric lifetime of 4.3 yr, Bunce et al. 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance \( t_\frac{1}{2} = 2.4–24 \text{ h} \) from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); lifetime of 44 yr in troposphere (Altshuller 1980); estimated tropospheric lifetime of 4.3 yr as global average for the reaction with hydroxyl radical in air (Bunce et al. 1991); estimated tropospheric lifetime of 7.5 yr and 15.8 yr by rigorous calculation (Nimitz & Skaggs 1992).
TABLE 5.1.4.4.1
Reported aqueous solubilities and vapor pressures of chlorodifluoromethane (HCFC-22) at various temperatures

\[
S/(\text{wt%}) = 0.8171 - 3.5818 \times 10^{-2} \cdot (t/°C) + 8.0081 \times 10^{-4} \cdot (t/°C)^2 - 1.0075 \times 10^{-5} \cdot (t/°C)^3 + 6.9823 \times 10^{-8} \cdot (t/°C)^4 \tag{1}
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>(S/\text{g} \cdot \text{m}^{-3})</th>
<th>(t/°C)</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>5296</td>
<td>-122.8</td>
<td>133.3</td>
</tr>
<tr>
<td>20</td>
<td>3510</td>
<td>-110.2</td>
<td>666.6</td>
</tr>
<tr>
<td>25</td>
<td>2899</td>
<td>-103.7</td>
<td>1333</td>
</tr>
<tr>
<td>30</td>
<td>2428</td>
<td>-96.5</td>
<td>2666</td>
</tr>
<tr>
<td>40</td>
<td>1783</td>
<td>-88.6</td>
<td>5333</td>
</tr>
<tr>
<td>50</td>
<td>1402</td>
<td>-83.4</td>
<td>7999</td>
</tr>
<tr>
<td>60</td>
<td>1180</td>
<td>-76.4</td>
<td>13332</td>
</tr>
<tr>
<td>70</td>
<td>1052</td>
<td>-65.8</td>
<td>26664</td>
</tr>
<tr>
<td>80</td>
<td>972.8</td>
<td>-53.6</td>
<td>53329</td>
</tr>
<tr>
<td>eq. 1</td>
<td>(S/(\text{wt%}))</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

mp/°C = -160.0

FIGURE 5.1.4.4.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for chlorodifluoromethane.
5.1.4.5 Dichlorodifluoromethane (CFC-12)

Common Name: Dichlorodifluoromethane
Synonym: difluorodichloromethane, Freon 12, CFC-12
Chemical Name: dichlorodifluoromethane
CAS Registry No: 75-71-8
Molecular Formula: CF₂Cl₂
Molecular Weight: 120.914

Melting Point (°C):
-158.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point (°C):
-29.8 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³ at 20°C):
1.3110 (25°C, Kirk-Othmer 1985)
1.3292, 1.3113 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
92.2 (Stephenson & Malanowski 1987)
81.4 (Stephenson & Malanowski 1987)
81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
20.112 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔHfus (kJ/mol):
4.14 (Riddick et al. 1986)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):
280 (DuPont 1966; quoted, Horvath 1982; Riddick et al. 1986)
276 (Gmelins 1974)
280 (shake flask-GC, Pearson & McConnell 1975)
300 (recommended, Horvath 1982)
280 (Verschueren 1983; Dean 1985; Kirk-Othmer 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
745000, 1031000 (20°C, 30°C, static method, Gilkey et al. 1931)
101325 (~−29.8°C, summary of literature data, temp range −118.5 to −29.8°C, Stull 1947)
214220 (calculated-Antoine eq., Weast 1975)

log (P/mmHg) = 6.82101 − 839.622/(t°C + 242.861); temp range −101 to +6°C (Antoine eq., Kudchadker et al. 1979)
566500, 769940 (20°C, 30°C, Verschueren 1983)
566600 (20°C, quoted, Riddick et al. 1986)

log (P/kPa) = 5.94591 − 839.622/(242.861 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
651040 (interpolated-Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/kPa) = 5.9477 − 839.6/(-30.311 + T/K); temp range 173–244 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.0058 − 860.828/(-28.11 + T/K); temp range 173–240 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 5.92289 − 826.707/(-32.274 + T/K); temp range 236–285 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 6.30541 − 1035.857/(-1.496 + T/K); temp range 282–345 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log \( P_{\text{mmHg}} \) = 52.5701 – 2.2537 \times 10^{3}/(T/K) – 18.265 \log (T/K) + 1.298 \times 10^{–2}/(T/K) + 2.0286 \times 10^{–13}/(T/K)^{2}; 
\text{temp range 115–385 K (vapor pressure eq., Yaws 1994)}

\text{log} \( P_{\text{kPa}} \) = 7.51271 – 2016.711/(132.578 + T/K); \text{temp range 341–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)}

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated):

151960 (calculated-P/C, Mackay & Wolkoff 1973; quoted, Roberts & Dändliker 1983)

43080 (calculated-1/K_{AW}, C_{W}/C_{A}, reported as exp.!, Hine & Mookerjee 1975)

22800 (estimated, Roberts 1984)

28704 (19.93°C, equilibrium cell-GC, measured range 0–40°C, Warner & Weiss 1985)

log \( K_{AW} \) = 5.811 – 1399/(T/K); \text{temp range: 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)}

304000 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)

39557 (computed value, Yaws et al. 1991)

26566 (20°C, selected from literature experimentally measured data, Staudeger & Roberts 1996)

26810 (20°C, selected from reported experimental determined values, Staudeger & Roberts 2001)

log \( K_{AW} \) = 5.739 – 1380/(T/K) (summary of literature data, Staudeger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

2.16 (shake flask-GC, Hansch et al. 1975)

2.21 (calculated-fragment const., Rekker & de Kort 1979)

2.16 (recommended, Sangster 1993)

2.16 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

2.05 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, \( k_{i} \), and Half-Lives, \( t_{1/2} \):

Volatilization: half-life of about few minutes (Mills et al. 1982); loss half-lives in marine mesocosm were estimated to be 20 d in spring at 8–16°C and \( t_{1/2} = 13 \) d in winter at 3–7°C (Wakeham et al. 1983).

Photolysis: photolytic dissociation of atmospheric CFCl_3 and CF_2Cl_2 gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3 or as indicated, *data at other temperatures see reference:

\( k_{OH} > 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 297.3 K, measured range 297–423.8 K (flash photolysis-RF, Atkinson et al. 1975)

\( k_{OH} > 0.4 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

\( k_{OH} < 0.012 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (relative rate method, Cox et al. 1976)

photooxidation \( t_{1/2} = 2118–21180 \) h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)

\( k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (Atkinson 1985)

\( k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with estimated tropospheric lifetime of > 50 yr for a global average concentration of OH radical (Bunce et al. 1991).

\( k_{OH} < 1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: aqueous aerobic \( t_{1/2} = 672–4320 \) h, based on acclimated aerobic screening test data for trichlorofluoromethane (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic \( t_{1/2} = 2688–16128 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (\( k_{1} \)) and Elimination (\( k_{2} \)) Rate Constants or Half-Lives:
Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); residence time of about 50 yr in N. troposphere, estimated by one-compartment nonsteady state model (Singh et al. 1978) and residence time of 60–70 yr by two-compartment nonsteady state model (Singh et al. 1979); estimated residence time in troposphere about 1 year (Lyman 1982);

$t_{1/2} = 2118–21180$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated global average tropospheric lifetime $\tau > 50$ yr for the reaction with hydroxyl radical in air (Bunce et al. 1991).

Surface water: $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344–8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated $t_{1/2} \sim 10000$ d for volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
Common Name: Trichlorofluoromethane
Synonym: Arcton 11, fluoro trifluoromethane, fluorocarbon-11, Freon-11, Frigen 11, R 11, CFC-11
Chemical Name: trichlorofluoromethane, fluorotrichloromethane
CAS Registry No: 75-69-4
Molecular Formula: CFCl₃
Molecular Weight: 137.368

Melting Point (°C): 
-110.44 (Lide 2003)

Boiling Point (°C): 
23.7 (Lide 2003)

Density (g/cm³ at 20°C):
1.4879, 1.4760 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
93.1 (Stephenson & Malanowski 1987)
97.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
25.02, 25.06 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
6.895 (Riddick et al. 1986)

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
1400 (21°C, Irmann 1965; Chiou & Freed 1977)
1100 (20°C, DuPont 1966; quoted, Riddick et al. 1986)
1100 (20°C, Pearson & McConnell 1975)
1100 (Verschueren 1977, 1983)
1080 (recommended, Horvath 1982)
1080 (30°C, Horvath 1982)
1400 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
88550* (19.895°C, measured range −36.673 to 19.895°C, Osborne et al. 1941)
log (P/mmHg) = 18.54101 − 1841.72/(T/K) − 3.8423.log (T/K); temp range 236.487–296.822 K (static method-manometry, Osborne et al. 1941)
101325* (23.7°C, summary of literature data, temp range −84.3 to 23.7°C, Stull 1947)
95670 (calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [−0.2185 × 6424.1/(T/K)] + 7.563786; temp range −84.3 to 13.1°C (Antoine eq., Weast 1972–73)
88500 (20°C, Pearson & McConnell 1975)
106390 (Antoine eq., Reid et al. 1977)
106349 (20°C, calculated-Antoine eq., Kudchadker et al. 1979)
log (P/mmHg) = 6.89396 − 1074.04/(t/°C + 237.276); temp range −37 to 20°C (Antoine eq., Kudchadker et al. 1979)
91580 (20°C, Verschueren 1983)
log (P/kPa) = 6.01333 − 1044.954/(237.102 + t/°C); temp range −36.67 to 19.89°C (Antoine eq. derived from exptl data of Osborne et al. 1941, Boublik et al. 1984)
107010 (Daubert & Danner 1985)
log (P/kPa) = 6.01886 – 1047.04/(237.276 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.99652 – 1034.048/(–37.672 + T/K); temp range 213–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.03083 – 1053.874/(–34.955 + T/K); temp range 295–363 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 6.36472 – 1285.088/(–0.653 + T/K); temp range 357–429 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/kPa) = 7.75501 – 2744.806/(196.225 + T/K); temp range 213–249 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (PL/kPa) = 6.03083 – 1053.874/(–34.955 + T/K); temp range 295–363 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

ln KAW = 9.25 – 2372/(T/K); measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

ln KAW = 10.50 – 2652/(T/K); measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)

ln KAW = 10.50 – 2652/(T/K); measured range 0–40°C, Warner & Weiss 1985

ln KAW = 9.480 – 3513/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

Octanol/Water Partition Coefficient, log Kow:
2.53 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)
2.53 (recommended, Sangster 1993)
2.53 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.92 (microorganisms-water, calculated-Kow, Mabey et al. 1982)
1.95 (calculated, Klöpffer et al. 1982)

Sorption Partition Coefficient, log Koc:
2.20 (sediment-water, calculated-Kow, Mabey et al. 1982)
2.31, 2.42, 2.16, 2.21 (estimated-Kow, Karickhoff 1985)
2.13, 2.26 (estimated-S, Karickhoff 1985)
2.20 (best estimate, Karickhoff 1985)
2.13 (average from estimates of Kow and S, Karickhoff 1985; quoted, Neely & Blau 1985)
Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization: estimated t½ = 3.4 h from Henry’s law constant for a river 1.0 m deep with a 3 m/s wind and 1 m/s current (Lyman et al. 1982; Cadena et al. 1984; quoted, Howard 1990); t½ ~ few minutes (Mills et al. 1982).

Photolysis: photolytic dissociation of atmospheric CFCl₃ and CF₂Cl₂ gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ as indicated, *data at other temperatures see reference:

\[ k_{OH} \leq 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296.8 \text{ K, measured range } 297–424 \text{ K (flash photolysis-resonance fluorescence, Atkinson et al. 1975)} \]
\[ k_{OH} < 0.05 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (discharge flow-LMR, Howard & Evenson 1976a)} \]
\[ k_{OH} < 0.005 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (relative rate method, Cox et al. 1976)} \]
\[ k_{OH} < 1.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)} \]

Hydrolysis: estimated exptl. rate constant k = 9.5 \times 10^{-7} \text{ d}^{-1}, based on carbon tetrachloride (Neely 1985).

Biodegradation: aqueous aerobic t½ = 4032–8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic t½ = 16128–34560 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Half-Lives in the Environment:

Air: disappearance t½ > 10 d from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976); estimated residence time about 1000 yr in troposphere for the reaction with OH radical (CEQ 1975); estimated residence time in N. troposphere about 15–20 yr by one-compartment nonsteady state model and 40–45 yr in troposphere by two-compartment nonsteady state model (Singh et al. 1979); estimated residence time in troposphere about 1–6 yr (Lyman 1982); t½ = 14.7–147 yr, based on an measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).


Ground water: t½ = 8640–17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: t½ = 4320–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
# Table 5.1.4.6.1

Reported vapor pressures and Henry's law constants of trichlorofluoromethane (CFC-11) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (P/Pa)</th>
<th>Henry's Law Constant (H/(Pa·m³/mol))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Osborne et al. 1941</td>
<td>Stull 1947</td>
</tr>
<tr>
<td>Static Method</td>
<td></td>
<td>EPICS-GC</td>
</tr>
<tr>
<td></td>
<td>Methods</td>
<td>Summary of Literature Data</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>–36.673</td>
<td>6313</td>
<td>–84.3</td>
</tr>
<tr>
<td>–21.825</td>
<td>14416</td>
<td>–67.6</td>
</tr>
<tr>
<td>–6.887</td>
<td>29811</td>
<td>–59.0</td>
</tr>
<tr>
<td>–2.352</td>
<td>44611</td>
<td>–49.7</td>
</tr>
<tr>
<td>–10.362</td>
<td>61790</td>
<td>–39.0</td>
</tr>
<tr>
<td>15.108</td>
<td>74147</td>
<td>–32.3</td>
</tr>
<tr>
<td>19.895</td>
<td>88550</td>
<td>–23.0</td>
</tr>
<tr>
<td>23.662</td>
<td>101325</td>
<td>–9.10</td>
</tr>
</tbody>
</table>

ln[H/(atm·m³/mol)] = A – B/(T/K)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (P/Pa)</th>
<th>Henry's Law Constant (H/(Pa·m³/mol))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Figure 5.1.4.6.1** Logarithm of Henry’s law constant versus reciprocal temperature for trichlorofluoromethane.
5.1.4.7 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)

\[
\begin{align*}
\text{Cl} & \quad \text{F} & \quad \text{Cl} \\
\text{F} & \quad \text{Cl} & \quad \text{F}
\end{align*}
\]

Common Name: 1,1,2-Trichloro-1,2,2-trifluoroethane  
Synonym: CFC-113, Freon 113, 1,2,2-trifluoro-1,1,2-trichloroethane  
Chemical Name: 1,1,2-trichloro-1,2,2-trifluoroethane, Ark lone  
CAS Registry No: 76-13-1  
Molecular Formula: C₂Cl₃F₃, CCIF₂CCl₂F  
Molecular Weight: 187.375  
Melting Point (°C):  
\(-36.22\)  
(\text{Lide 2003})  
Boiling Point (°C):  
\(47.7\)  
(\text{Lide 2003})  
Density (g/cm³ at 20°C):  
\(1.5635\)  
(\text{25°C, Dean 1985; Riddick et al. 1986})  
Molar Volume (cm³/mol):  
\(119.8\)  
(\text{20°C, calculated-density})  
\(129.5\)  
(\text{calculated-Le Bas method at normal boiling point})  
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):  
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):  
\(170\)  
(\text{DuPont 1966; quoted, Riddick et al. 1986})  
\(170\)  
(\text{shake flask-GC, Rauws et al. 1973})  
\(170\)  
(\text{20°C, Jones et al. 1977/1978})  
\(166.4^*\)  
(\text{summary of literature data, Horvath 1982})  
\(170\)  
(\text{Dean 1985})  
\(170\)  
(\text{recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a})  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):  
\(53329^*\)  
(\text{30.2°C, summary of literature data, temp range –68.0 to 47.4°C, Stull 1947})  
\(48476^*\)  
(\text{static method-isoteniscope, measured range 273.35–318.10 K, Hiraoka & Hildebrand 1963})  
\(39040\)  
(\text{calculated-Antoine eq., Weast 1972–73})  
\(48320\)  
(\text{calculated-Antoine eq., Boublik et al. 1984})  
\(48480\)  
(\text{selected, Riddick et al. 1986})  
\(\log (P/kPa) = 6.6783 – 1499.2/(T/K),\) temp range not specified (Antoine eq., Riddick et al. 1986)  
\(\log (P_{L}/kPa) = 5.91657 – 1094.37/(–39.61 + T/K);\) temp range 273–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
\(\log (P/kPa) = 6.01641 – 1115.812/(–42.515 + T/K);\) temp range 238–364 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
\(\log (P_{L}/kPa) = 6.53093 – 1500.489/(12.469 + T/K);\) temp range 360–473 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
\(\log (P/kPa) = 5.95163 – 1082.588/(46.427 + T/K);\) temp range 297–317 K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
\(\log (P/mmHg) = 33.7911 – 2.5323 \times 10^{19}/(T/K) – 9.3175 \times 10^{4}/(T/K) + 1.455 \times 10^{5}/(T/K) + 2.914 \times 10^{6}/(T/K)^{2};\) temp range 238–481 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 32320* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
- \( \ln \frac{[H/(atm \cdot m^3/mol)]}{T/K} = 9.649 - \frac{3243}{T/K} \); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 53300 (calculated-P/C, Howard 1990)
- 49132 (computed value, Yaws et al. 1991)
- 24616 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

- \( \log K_{AW} = 5.375 - \frac{1281}{T/K} \) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

- 3.16 (HPLC-k correlation, McDuffie 1981; quoted, Howard 1990, Sangster 1993))
- 3.16 (recommended, Hansch et al. 1995)

Bioconcentration Factor, \( \log BCF \):

- 1.531, 1.041 (calculated-S, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, \( \log K_{OC} \):

- 2.28, 2.41 (soil, calculated-K_{OW}, calculated-S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

- Volatilization: using Henry’s law constant, \( t_{1/2} = 4 \) h was estimated for a model river 1 m deep flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).
- Photolysis: both aqueous and atmospheric photolysis half-lives are infinite (Howard et al. 1991).
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃, as indicated, *data at other temperatures see reference:
  - \( k_{OH} < 0.3 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K (discharge flow-laser magnetic resonance, Howard & Enenson 1976b)
  - photooxidation \( t_{1/2} = 40–1000 \) yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991).
- Hydrolysis:
- Biodegradation: aqueous aerobic \( t_{1/2} = 4320–8640 \) h, based on a relative resistance of completely halogenated aliphatics to biodegrade; aqueous anaerobic \( t_{1/2} = 17280–34560 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); degradation rates in microcosms at 20°C: \( k = 7.6 \times 10^{-3} \text{ d}^{-1} \) by control buffer with \( t_{1/2} = 90 \) d, \( k = 9.1 \times 10^{-3} \text{ d}^{-1} \) by redox buffer with \( t_{1/2} = 75 \) d, \( k = 1.2 \times 10^{-3} \text{ d}^{-1} \) by 1 mg/L redox-hematin with \( t_{1/2} = 57 \) d, \( k = 1.6 \times 10^{-2} \text{ d}^{-1} \) by 2 mg/L redox-hematin with \( t_{1/2} = 43 \) d, \( k = 9.9 \times 10^{-2} \text{ d}^{-1} \) by purged leachate with \( t_{1/2} = 7 \) d, and \( k = 0.14 \text{ d}^{-1} \) by leachate with \( t_{1/2} = 5 \) d (Lesage et al. 1992).

- Biotransformation:
- Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

- Half-Lives in the Environment:
- Air: disappearance \( t_{1/2} > 10 \) d from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976); \( t_{1/2} = 40–1000 \) yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991); \( t_{1/2} = 20 \) yr in troposphere (Dilling 1982; quoted, Howard 1990).
- Surface water: \( t_{1/2} = 4320–8640 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Ground water: \( t_{1/2} = 1440–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment:
- Soil: \( t_{1/2} = 4320–8640 \) h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).
- Biota:
TABLE 5.1.4.7.1
Reported aqueous solubilities, vapor pressures and Henry's law constants of 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113) at various temperatures

\[
S/(\text{wt}%) = 1.0648 \times 10^{-2} + 3.51135 \times 10^{-4}(t/\degree\text{C}) - 6.1331 \times 10^{-6}(t/\degree\text{C})^2 + 6.70235 \times 10^{-8}(t/\degree\text{C})^3 \quad (1)
\]

\[
\ln \left[ \frac{H}{\text{atm} \cdot \text{m}^3/\text{mol}} \right] = A - \frac{B}{T/\text{K}} \quad (2)
\]

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>summary of literature data</td>
<td>summary of literature data</td>
<td>static method isoteniscope</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m (^{-3})</td>
<td>t/°C</td>
</tr>
<tr>
<td>-----</td>
<td>----------------</td>
<td>-----</td>
</tr>
<tr>
<td>0</td>
<td>106.5</td>
<td>-68.0</td>
</tr>
<tr>
<td>10</td>
<td>136.1</td>
<td>-49.4</td>
</tr>
<tr>
<td>20</td>
<td>157.5</td>
<td>-40.3</td>
</tr>
<tr>
<td>25</td>
<td>166.4</td>
<td>-30.0</td>
</tr>
<tr>
<td>30</td>
<td>174.7</td>
<td>-18.5</td>
</tr>
<tr>
<td>40</td>
<td>191.7</td>
<td>-11.2</td>
</tr>
<tr>
<td>50</td>
<td>212.5</td>
<td>-1.70</td>
</tr>
<tr>
<td>60</td>
<td>241.1</td>
<td>13.5</td>
</tr>
<tr>
<td>70</td>
<td>281.6</td>
<td>30.2</td>
</tr>
<tr>
<td>80</td>
<td>338.0</td>
<td>47.4</td>
</tr>
</tbody>
</table>

eq.1 \( S/\text{wt}\% \)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>mp/°C</th>
<th>-35</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,1,2-Trichloro-1,2,2-trifluoroethane: solubility vs. 1/T</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 5.1.4.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.
FIGURE 5.1.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

FIGURE 5.1.4.7.3 Logarithm of Henry’s law constant versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.
5.1.4.8  1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)

Common Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane
Synonym: Freon-112, CFC-112
Chemical Name: 1,2-difluorotetrachloroethane
CAS Registry No: 76-12-0
Molecular Formula: C_2F_2Cl_4, Cl_2FCCFCl_2
Molecular Weight: 203.830

Melting Point (°C):
- 26.55  (Riddick et al. 1986)
- 24.9   (Lide 2003)

Boiling Point (°C):
- 92.80  (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at 20°C):
- 1.6447  (25°C, Riddick et al. 1986)

Molar Volume (cm^3/mol):
- 145.4   (calculated-Le Bas method at normal boiling point)

Enthalpy of vaporization, \( \Delta H_v \) (kJ/mol):
- 35      (Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
- 3.666   (Riddick et al. 1986)

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
- 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
- 120    (DuPont 1966; quoted, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 6106   (20°C, measured range 10–91.5°C, Hovorka & Geiger 1933)
- 7609   (calculated-Antoine eq., Boublik et al. 1984)
- \log (P/kPa) = 9.94341 – 4259.092/(444.991 + \theta°C), temp range 10–91.5°C (Antoine eq. derived from exptl. data of Hovorka & Geiger 1933, Boublik et al. 1984)
- 8770   (selected, Riddick et al. 1986)
- \log (P/kPa) = 7.2972 – 1929.27/(T/K); temp range not specified (Antoine eq., Riddick et al. 1986)
- \log (P/kPa) = 6.50788 – 1526.24/(–28.93 + T/K); temp range 235–293 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
- \log (P/kPa) = 6.67780 – 1567.8/(–29.58 + T/K); temp range 301–365 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- \log (P/kPa) = 5.97313 – 1239.993/(–53.468 + T/K); temp range 312–362 K (Antoine eq., Stephenson & Malanowski 1987)
- \log (P/mmHg) = –38.1282 – 1.2604 \times 10^{-2} (T/K) + 23.347 \times \log (T/K) – 3.4436 \times 10^{-2} (T/K) + 1.7407 \times 10^{-5} (T/K)^2; temp range 299–551 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
- 9869   (calculated-I/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
- 248, 1426 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 161419 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- 2.82   (shake flask, Log P Database, Hansch & Leo 1987)
- 3.73   (Howard 1990)
- 2.82   (recommended, Sangster 1993)
Bioconcentration Factor, log BCF:
1.62 (estimated-S, Lyman et al. 1982)

Sorption Partition Coefficient, log $K_{OC}$:
2.50 (soil, estimated-linear regression with S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:
Volatilization: volatilization $t_\text{1/2} \approx 4.0$ h from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s, based on estimated Henry's law constant (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).
Photolysis: will not undergo direct photolysis in the troposphere (quoted, Howard 1990).
Hydrolysis: not an environmentally significant fate process (DuPont 1980; quoted, Howard 1990).
Biodegradation:
Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: by analogy to other Freon compounds, Freon-112 is predicted to have a stratospheric lifetime on the order of several decades (Chou et al. 1978; quoted, Howard 1990).
Surface water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).
Ground water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).
Sediment: will volatilize very rapidly from soil surfaces (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).
Soil:
Biota:
5.1.5  FLUOROALKANES AND FLUOROALKENES

A large number of stable and volatile fluorinated and chlorinated alkanes and alkenes have been synthesized and used, primarily as refrigerants. These “freons” have been implicated as the cause of observed reductions in stratospheric ozone levels, thus permitting greater penetration of ultraviolet radiation to the Earth’s surface. Their high vapor pressures and relatively low solubilities in water result in high Henry’s law constants or air-water partition coefficients. Fate calculations show that when released into the environment virtually the total mass of these substances will partition to the atmospheric compartment. Levels in water, soil, sediments and biota are likely to be very low and of little concern. Accordingly, there is little merit in compiling detailed data on these substances in a format comparable to that, for example, the chlorobenzenes or PCBs.

In the interest of conserving space in this handbook, a compact tabular presentation format has been adopted. Table 5.1.5.1 lists the chemical name, and its freon number (if applicable), molecular formula, molar weight and melting and boiling points. These data are available for virtually all substances in this group. Also shown in this table is the availability, expressed as a tick mark, of data on vapor pressure, solubility in water, octanol-water partition coefficient (K_{OW}) and the second order reaction rate constant with hydroxyl radicals. This rate constant is the critical determinant of persistence in the atmosphere. Tables 5.1.5.2 to 5.1.5.5 list the compounds and give the available property data with citations.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Freon no.</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight g/mol</th>
<th>mp°C</th>
<th>bp°C</th>
<th>Le Bas molar volume, $V_M$ cm$^3$/mol</th>
<th>Properties**</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluoroalkanes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoromethane</td>
<td>HFC-41</td>
<td>593-53-3</td>
<td>CH$_3$F</td>
<td>34.05</td>
<td>-141.8</td>
<td>-79.1</td>
<td>34.6</td>
<td>✓</td>
</tr>
<tr>
<td>Difluoromethane</td>
<td>HFC-32</td>
<td>75-10-5</td>
<td>CH$_2$F$_2$</td>
<td>52.02</td>
<td>-136</td>
<td>-51.6</td>
<td>39.6</td>
<td>✓</td>
</tr>
<tr>
<td>Trifluoromethane</td>
<td>HFC-23</td>
<td>75-46-7</td>
<td>CHF$_3$</td>
<td>70.01</td>
<td>-155.2</td>
<td>-82.16</td>
<td>44.6</td>
<td>✓</td>
</tr>
<tr>
<td>Tetrafluoromethane</td>
<td>FC-14</td>
<td>75-73-0</td>
<td>CF$_4$</td>
<td>88.005</td>
<td>-183.60</td>
<td>-128.0</td>
<td>49.6</td>
<td>✓</td>
</tr>
<tr>
<td>Chlorofluoromethane</td>
<td>HCFC-31</td>
<td>593-70-4</td>
<td>CH$_2$ClF</td>
<td>68.48</td>
<td>-133</td>
<td>-9.1</td>
<td>55.5</td>
<td>✓</td>
</tr>
<tr>
<td>Dichlorofluoromethane</td>
<td>HCFC-21</td>
<td>75-43-4</td>
<td>CHClF$_2$</td>
<td>102.92</td>
<td>-135</td>
<td>8.92</td>
<td>76.4</td>
<td>✓</td>
</tr>
<tr>
<td>Chlorodifluoromethane</td>
<td>HCFC-22*</td>
<td>75-45-6</td>
<td>CHClF$_2$</td>
<td>86.47</td>
<td>-160</td>
<td>-40.7</td>
<td>60.5</td>
<td>✓</td>
</tr>
<tr>
<td>Chlorotrifluoromethane</td>
<td>FC-13</td>
<td>75-72-9</td>
<td>CF$_3$Cl</td>
<td>104.46</td>
<td>-181</td>
<td>-82</td>
<td>65.5</td>
<td>✓</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>CFC-12*</td>
<td>75-71-8</td>
<td>CFCl$_2$F$_2$</td>
<td>120.91</td>
<td>-155</td>
<td>-29.8</td>
<td>81.4</td>
<td>✓</td>
</tr>
<tr>
<td>Trichlorodifluoromethane</td>
<td>CFC-11*</td>
<td>75-69-4</td>
<td>CFCl$_3$F$_2$</td>
<td>137.37</td>
<td>-111</td>
<td>23.82</td>
<td>97.3</td>
<td>✓</td>
</tr>
<tr>
<td>Fluoroethane</td>
<td>HFC-161</td>
<td>353-36-6</td>
<td>CH$_3$CH$_2$F</td>
<td>48.06</td>
<td>-143</td>
<td>-37.7</td>
<td>56.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,1-Difluoroethane</td>
<td>HFC-152a</td>
<td>75-37-6</td>
<td>CH$_3$CHF$_2$</td>
<td>66.05</td>
<td>-117</td>
<td>-24.7</td>
<td>61.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,2-Difluoroethane</td>
<td>HFC-152</td>
<td>624-72-6</td>
<td>CH$_2$FCH$_2$F</td>
<td>66.05</td>
<td></td>
<td>26</td>
<td>61.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,1-Trifluoroethane</td>
<td>HFC-143a</td>
<td>420-46-2</td>
<td>CF$_3$CH$_2$</td>
<td>84.04</td>
<td>-111.3</td>
<td>-47.4</td>
<td>66.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,2-Trifluoroethane</td>
<td>HFC-143b</td>
<td>430-66-0</td>
<td>CH$_2$FCHF$_3$</td>
<td>84.04</td>
<td>-84</td>
<td>3.7</td>
<td>66.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,2,2-Tetrafluoroethane</td>
<td>HFC-134</td>
<td>359-35-3</td>
<td>CHF$_2$CHF$_3$</td>
<td>102.03</td>
<td>-89</td>
<td>-19.9</td>
<td>71.8</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,1,2-Tetrafluoroethane</td>
<td>HFC-134a</td>
<td>811-97-2</td>
<td>CH$_3$CF$_2$F$_2$</td>
<td>102.03</td>
<td>-103.3</td>
<td>-26.08</td>
<td>71.8</td>
<td>✓</td>
</tr>
<tr>
<td>Pentafluoroethane</td>
<td>HFC-125</td>
<td>354-33-6</td>
<td>CF$_3$CHF$_3$</td>
<td>120.02</td>
<td>-103</td>
<td>-48.5</td>
<td>76.8</td>
<td>✓</td>
</tr>
<tr>
<td>Hexafluoroethane</td>
<td>FC-116</td>
<td>76-16-4</td>
<td>CF$_3$CF$_3$</td>
<td>138.01</td>
<td>-100.6</td>
<td>-79</td>
<td>81.8</td>
<td>✓</td>
</tr>
<tr>
<td>1-Chloro-2-fluoroethane</td>
<td>HCFC-151</td>
<td>762-50-5</td>
<td>CH$_2$FCH$_2$Cl</td>
<td>82.5</td>
<td>-50</td>
<td>52.8</td>
<td>77.7</td>
<td>✓</td>
</tr>
<tr>
<td>1-Chloro-1,1-difluoroethane</td>
<td>HCFC-142b</td>
<td>75-68-3</td>
<td>CH$_3$CCIF$_2$</td>
<td>100.5</td>
<td>-130.8</td>
<td>-9.5</td>
<td>82.7</td>
<td>✓</td>
</tr>
<tr>
<td>1-Chloro-1,1,2-trifluoroethane</td>
<td>HCFC-133a</td>
<td>421-04-5</td>
<td>CH$_2$CCIF$_3$</td>
<td>118.49</td>
<td>12</td>
<td>87.7</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,2,2,2-tetrafluoroethane</td>
<td>HCFC-124</td>
<td>2837-89-0</td>
<td>CHClF$_2$CF$_3$</td>
<td>136.5</td>
<td>-11.0</td>
<td>92.7</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>1-Chloropentafluoroethane</td>
<td>CFC-115</td>
<td>76-15-3</td>
<td>CClF$_3$CF$_3$</td>
<td>154.47</td>
<td>-99.4</td>
<td>-39.1</td>
<td>97.7</td>
<td>✓</td>
</tr>
<tr>
<td>1,1-Dichloro-1-fluoroethane</td>
<td>HCFC-141b</td>
<td>1717-00-6</td>
<td>CCl$_3$CHF$_3$</td>
<td>116.95</td>
<td>-103.5</td>
<td>32.0</td>
<td>98.6</td>
<td>✓</td>
</tr>
<tr>
<td>1,2-Dichloro-1,1-difluoroethane</td>
<td>HCFC-132b</td>
<td>1649-08-7</td>
<td>CClF$_2$CH$_2$Cl</td>
<td>134.97</td>
<td>-101.2</td>
<td>46.8</td>
<td>103.6</td>
<td>✓</td>
</tr>
<tr>
<td>1,1-Dichlorotrifluoroethane</td>
<td>HCFC-123</td>
<td>306-83-2</td>
<td>CHClF$_3$</td>
<td>152.93</td>
<td>-107</td>
<td>27.6</td>
<td>108.6</td>
<td>✓</td>
</tr>
<tr>
<td>1,2-Dichloro-1,1,2,2-tetrafluoroethane</td>
<td>CFC-114</td>
<td>76-14-2</td>
<td>CClF$_3$CCIF$_3$</td>
<td>170.92</td>
<td>-93.9</td>
<td>3.8</td>
<td>113.6</td>
<td>✓</td>
</tr>
<tr>
<td>1,1-Dichloro-1,2,2,2-tetrafluoroethane</td>
<td>CFC-114a</td>
<td>374-07-2</td>
<td>CCl$_3$F$_3$CF$_3$</td>
<td>170.92</td>
<td>-56.6</td>
<td>3.4</td>
<td>113.6</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,1-Trichloro-2,2,2-trifluoroethane</td>
<td>CFC-113a</td>
<td>354-58-5</td>
<td>CCl$_3$CF$_3$</td>
<td>187.38</td>
<td>14.2</td>
<td>47.57</td>
<td>129.5</td>
<td>✓</td>
</tr>
<tr>
<td>1,1,2-Trichloro-1,2,2-trifluoroethane</td>
<td>CFC-113*</td>
<td>76-13-1</td>
<td>CCl$_3$FCCIF$_3$</td>
<td>187.38</td>
<td>-36.4</td>
<td>47.7</td>
<td>129.5</td>
<td>✓</td>
</tr>
<tr>
<td>Compound</td>
<td>Formula</td>
<td>CAS Number</td>
<td>Molecular Weight</td>
<td>Density @ 20°C</td>
<td>Viscosity @ 20°C</td>
<td>VPO (ppm)</td>
<td>Critical Temperature</td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>---------</td>
<td>------------</td>
<td>-----------------</td>
<td>---------------</td>
<td>----------------</td>
<td>-----------</td>
<td>---------------------</td>
<td></td>
</tr>
<tr>
<td>1,1-Difluorotetrachloroethane</td>
<td>CCl₂FCCl₂</td>
<td>1211</td>
<td>203.83</td>
<td>38</td>
<td>91</td>
<td>145.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,2,2-tetrafluoro-1,2-difluoroethane</td>
<td>CCl₂FCCl₂F</td>
<td>1212</td>
<td>203.83</td>
<td>25</td>
<td>93</td>
<td>145.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-Fluoropropene</td>
<td>CH₂CHFCH₂</td>
<td>199</td>
<td>46.05</td>
<td>–160</td>
<td>–72.2</td>
<td>49.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3-Fluoropropene</td>
<td>CH₂CHFCH₂</td>
<td>355</td>
<td>60.07</td>
<td>–0.5</td>
<td>71.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexafluoropropene</td>
<td>CH₃CF₂CF₃</td>
<td>460</td>
<td>152.04</td>
<td>–93.6</td>
<td>–16.4</td>
<td>109.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* See Section 5.1.4. Mixed halogenated hydrocarbons.
** S = water solubility; P = vapor pressure; K<sub>OW</sub> = octanol-water partition coefficient; k<sub>OH</sub> = second order reaction rate constant with hydroxyl radicals.
### TABLE 5.1.5.2
Aqueous solubilities for fluoroalkanes and fluoroalkenes

<table>
<thead>
<tr>
<th>Compound</th>
<th>Temp.°C</th>
<th>Solubility</th>
<th>Unit</th>
<th>Range, wt %</th>
<th>Mole fraction x</th>
<th>Temp./pressure range</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluoroalkanes</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoromethane</td>
<td>25</td>
<td>0.2001</td>
<td>wt %</td>
<td>0.4227–0.08005</td>
<td>0.001061</td>
<td>0–80°C, 1 atm partial pressure</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>2390</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>4390</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Difluoromethane</td>
<td>25</td>
<td>0.09</td>
<td>g/100 mL</td>
<td>0.09–0.02</td>
<td></td>
<td>25–75°C, pressure 1–20.41 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.4087</td>
<td>wt %</td>
<td></td>
<td></td>
<td>1 atm partial pressure</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>900</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.0733</td>
<td>g/100 mL</td>
<td></td>
<td></td>
<td>from Hine &amp; Mookerjee (1975)</td>
<td>3</td>
</tr>
<tr>
<td>Trifluoromethane</td>
<td>25</td>
<td>0.001877</td>
<td>wt %</td>
<td>0.003892–0.001300</td>
<td>3.84×10⁻⁶</td>
<td>0–50°C, 1 atm partial pressure</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.00160</td>
<td>g/100 mL</td>
<td>0.00160–0.0005</td>
<td></td>
<td>25–75°C, 1–10.2 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>16.0</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.4592</td>
<td>10⁻³L₂,</td>
<td></td>
<td></td>
<td>288–303 K, 1 atm partial pressure</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>1.0522</td>
<td>wt %</td>
<td>1.6840–0.3285</td>
<td>0.002790</td>
<td>10–50°C, 1 atm partial pressure</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>10500</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td>1 atm partial pressure</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>1.8800</td>
<td>g/100 mL</td>
<td>1.88–0.418</td>
<td></td>
<td>25–75°C, 0.068–3.40 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.95</td>
<td>wt %</td>
<td></td>
<td></td>
<td>DuPont</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>18800</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.2899</td>
<td>wt %</td>
<td>0.5296–0.09728</td>
<td>6.055×10⁻⁴</td>
<td>10–50°C, 1 atm partial pressure</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.277</td>
<td>g/100 mL</td>
<td>0.792–0.089</td>
<td></td>
<td>5–76.7°C, 1–33.34 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.30</td>
<td>wt %</td>
<td></td>
<td></td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>27.7</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.2899</td>
<td>g/100 mL</td>
<td></td>
<td></td>
<td>from Horvath (1982)</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.009</td>
<td>g/100 mL</td>
<td>0.009–0.004</td>
<td></td>
<td>25–75°C, 1–23.81 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.009</td>
<td>wt %</td>
<td></td>
<td></td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>90</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>2.253</td>
<td>10⁻³L₂,</td>
<td></td>
<td></td>
<td>288–303 K, 1 atm partial pressure</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.030</td>
<td>g/100 mL</td>
<td>0.030–0.008</td>
<td></td>
<td>25–76.7°C, 1–6.80 atm</td>
<td>1</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>25</td>
<td>0.028</td>
<td>wt %</td>
<td></td>
<td></td>
<td>quoted Riddick (1986)</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.028</td>
<td>g/100 mL</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>300</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>7.110</td>
<td>10⁻³L₂,</td>
<td></td>
<td></td>
<td>288–303 K, 1 atm partial pressure</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.009</td>
<td>g/100 mL</td>
<td>0.108–0.031</td>
<td></td>
<td>25–75°C, 1–3.4 atm</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.11</td>
<td>wt %</td>
<td></td>
<td></td>
<td>DuPont</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>1080</td>
<td>ppm (wt)</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Compound</td>
<td>Concentration</td>
<td>Temperature</td>
<td>Pressure</td>
<td>From</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>----------------------------------</td>
<td>-----------------------</td>
<td>-------------</td>
<td>-------------------</td>
<td>---------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoroethane</td>
<td>0.108 g/100 mL</td>
<td>14–25°C</td>
<td>1 atm partial</td>
<td>Horvath (1982)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Difluoroethane</td>
<td>0.2158 wt %</td>
<td>0–27.5°C</td>
<td>1 atm partial</td>
<td>Horvath (1982)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2-Difluoroethane</td>
<td>0.0157 wt %</td>
<td>25–80°C</td>
<td>Saturation</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,2-Trifluoroethane</td>
<td>0.01664 wt %</td>
<td>0–27°C</td>
<td>Saturated</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,1,2-Tetrafluoroethane</td>
<td>0.00101 g/100 mL</td>
<td>30–75°C</td>
<td>0.34–2.04 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloro-2-fluoroethane</td>
<td>2.4390 wt %</td>
<td>287–328 K</td>
<td>96.6–120.5 kPa</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,1-difluoro-3</td>
<td>0.005429 wt %</td>
<td>1 atm partial</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,2,2,2-tetrafluoro-3</td>
<td>0.00058 g/100 mL</td>
<td>25–75°C</td>
<td>1–6.80 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloro-1-fluoro</td>
<td>0.066 wt %</td>
<td>25–80°C</td>
<td>0.068–0.612 atm</td>
<td>Riddick (1986)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Dichlorotrifluoroethane</td>
<td>0.0046 wt %</td>
<td>25–80°C</td>
<td>0.068–0.612 atm</td>
<td>Riddick (1986)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2-Dichloro-1,1,2,2-tetra-2</td>
<td>0.009 g/100 mL</td>
<td>30–75°C</td>
<td>0.068–0.612 atm</td>
<td>Riddick (1986)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloro-1,2,2,2-tetra-3</td>
<td>0.1100 wt %</td>
<td>0–27°C</td>
<td>1 atm partial</td>
<td>Horvath (1982)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,2-Trichloro-1,2,2-tri-4</td>
<td>0.01664 wt %</td>
<td>0–27°C</td>
<td>1 atm partial</td>
<td>Horvath (1982)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>30–75°C</td>
<td>0.34–2.04 atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th>Compound</th>
<th>Temp.°C</th>
<th>Solubility</th>
<th>Unit</th>
<th>Range, wt %</th>
<th>Mole fraction x</th>
<th>Temp./pressure range</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-Difluorotetrachloro-</td>
<td>25</td>
<td>0.012</td>
<td>wt %</td>
<td></td>
<td></td>
<td>from Riddick (1986)</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.012</td>
<td>g/100 mL</td>
<td></td>
<td></td>
<td></td>
<td>9</td>
</tr>
<tr>
<td>2-Fluoropropane</td>
<td>15</td>
<td>0.3663</td>
<td>wt %</td>
<td>0.001066</td>
<td>1 atm partial pressure</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>3660</td>
<td>ppm (wt)</td>
<td>1 atm partial pressure</td>
<td></td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Octafluoropropane</td>
<td>15</td>
<td>0.001495</td>
<td>wt %</td>
<td>1.432×10⁻⁶</td>
<td>15°C, saturated pressure</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Perfluorocyclobutane</td>
<td>21</td>
<td>0.014</td>
<td>wt %</td>
<td>1.259×10⁻⁶</td>
<td>21°C, 1 atm partial pressure</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>0.005</td>
<td>g/100 mL</td>
<td>0–37.8°C, 1–2.72 atm</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>50.0</td>
<td>ppm (wt)</td>
<td>0–37.8°C, 1–2.72 atm</td>
<td></td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Fluoroalkenes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Fluoroethylene</td>
<td>80 at 34 atm</td>
<td>0.9312</td>
<td>wt %</td>
<td>0.003664</td>
<td>34 atm</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>80 at 68 atm</td>
<td>1.5166</td>
<td>wt %</td>
<td>0.005988</td>
<td>68 atm</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>1,1-Difluoroethene</td>
<td>25</td>
<td>0.01649</td>
<td>wt %</td>
<td>4.638×10⁻⁵</td>
<td>1 atm partial pressure</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>165</td>
<td>ppm (wt)</td>
<td>1 atm partial pressure</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Tetrafluoroethene</td>
<td>25</td>
<td>0.01585</td>
<td>wt %</td>
<td>0.04062-0.008782</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>23 at 4.4 atm</td>
<td>0.001</td>
<td>wt %</td>
<td>0.001–1.274</td>
<td>0–70°C, 1 atm partial pressure</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>158</td>
<td>ppm (wt)</td>
<td>23°C, total pressure 4.4–13.45 atm</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>3-Fluoropropene</td>
<td>13</td>
<td>0.007167</td>
<td>wt %</td>
<td>2.149×10⁻⁵</td>
<td>1 atm partial pressure</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Hexafluoropropene</td>
<td>25</td>
<td>0.01691</td>
<td>wt %</td>
<td>2.327×10⁻⁵</td>
<td>0–70°C, 1 atm partial pressure</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

References:
<table>
<thead>
<tr>
<th>Compound</th>
<th>Temp. <em>°C or K</em></th>
<th>P* kPa</th>
<th>Method*</th>
<th>Temp. Range**</th>
<th>Pressure Range kPa</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluoroalkanes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoromethane</td>
<td></td>
<td></td>
<td>static</td>
<td>−103 − −76°C</td>
<td>20−116</td>
<td>Moles and Batuecas 1919*</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>literature summary</td>
<td>−133.1 − −87.5°C</td>
<td>1.33−101</td>
<td>Grosse et al. 1940</td>
</tr>
<tr>
<td></td>
<td>15.28°C</td>
<td>3045.3</td>
<td>manometer</td>
<td>−109−15°C</td>
<td>13−3045</td>
<td>Michels and Wassenaar 1948</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>3824.9</td>
<td>literature summary</td>
<td>131−317 K</td>
<td>0.43−5880</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>15.28°C</td>
<td>3045.3</td>
<td>literature summary</td>
<td>208−237 K</td>
<td>49−214</td>
<td>Weber and Goodwin 1993</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>1690.81</td>
<td>Burnett apparatus/densimeter</td>
<td>268−348 K</td>
<td>690−5409</td>
<td>Delfibaugh et al. 1994</td>
</tr>
<tr>
<td>Difluoromethane</td>
<td>298.16 K</td>
<td>1689</td>
<td>static</td>
<td>191−352 K</td>
<td>16.36−5828</td>
<td>Malbrunot et al. 1968</td>
</tr>
<tr>
<td></td>
<td>298.174 K</td>
<td>1690.81</td>
<td>comparative ebulliometry</td>
<td>208−237 K</td>
<td>49−214</td>
<td>Weber and Goodwin 1993</td>
</tr>
<tr>
<td></td>
<td>298.174 K</td>
<td>1690.81</td>
<td>Burnett apparatus/densimeter</td>
<td>268−348 K</td>
<td>690−5409</td>
<td>Delfibaugh et al. 1994</td>
</tr>
<tr>
<td></td>
<td>299.985 K</td>
<td>1774</td>
<td>manometer/densimeter</td>
<td>220−325 K</td>
<td>95−3278</td>
<td>Weber and Silva 1994</td>
</tr>
<tr>
<td></td>
<td>297.15 K</td>
<td>1645.1</td>
<td>Burnett apparatus</td>
<td>233−351 K</td>
<td>177−5767.9</td>
<td>Fu et al. 1995</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>1689.7</td>
<td>literature summary</td>
<td>137−351 K</td>
<td>5.69×10^{-2}−5780</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>308.15 K</td>
<td>2191</td>
<td>VLE</td>
<td></td>
<td></td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>4714.9</td>
<td>calorimetry static</td>
<td>145−192 K</td>
<td>2.72−102.51</td>
<td>Valentine et al. 1962</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>4714.9</td>
<td>literature summary</td>
<td>118−299 K</td>
<td>5.71×10^{-3}−4800</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>4714.9</td>
<td>literature summary</td>
<td>−184.6 − −127.7°C</td>
<td>0.1333−101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>calorimetry static</td>
<td>115−146 K</td>
<td>7−106</td>
<td>Smith and Pace 1969</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>literature summary</td>
<td>90−228 K</td>
<td>1.04×10^{-1}−3740</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>literature summary</td>
<td>138−427 K</td>
<td>2.28×10^{-3}−5700</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>isotensicopic</td>
<td>−29.65−174.6°C</td>
<td>17.31−4894</td>
<td>Benning and McHarness 1940</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>literature summary</td>
<td>−91.3−89.0°C</td>
<td>0.1333−101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td>298.15 K</td>
<td>181.67</td>
<td>literature summary</td>
<td>138−452 K</td>
<td>2.94×10^{2}−5183</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>22.6°C</td>
<td>951</td>
<td>manometer</td>
<td>22.6−96.4°C</td>
<td>951−4912</td>
<td>Booth and Swinehart 1935</td>
</tr>
<tr>
<td></td>
<td>25.15°C</td>
<td>1050.74</td>
<td>isotensicopic</td>
<td>−61.26−92.6°C</td>
<td>35.12−4652.84</td>
<td>Benning and McHarness 1940</td>
</tr>
<tr>
<td></td>
<td>50°C</td>
<td>1955</td>
<td>VLE</td>
<td></td>
<td>0.1333−101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td>65°C</td>
<td>2710</td>
<td>VLE</td>
<td></td>
<td></td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>70°C</td>
<td>3003</td>
<td>VLE</td>
<td></td>
<td></td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>75°C</td>
<td>3843</td>
<td>VLE</td>
<td></td>
<td></td>
<td>Xiang 2002</td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th>Compound</th>
<th>Temp. °C or K</th>
<th>P(^{\circ}) kPa</th>
<th>Method*</th>
<th>Temp. Range** °C or K</th>
<th>Pressure Range kPa</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorotrifluoromethane</td>
<td>289.10</td>
<td>811.7</td>
<td>isochoric</td>
<td>245–328</td>
<td>180–2195</td>
<td>Giuliani et al. 1995a</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>1044.2</td>
<td>literature summary</td>
<td>115–369</td>
<td>4.26×10(^{-4})–4988</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>3578.3</td>
<td>literature summary</td>
<td>–149.5––81.2°C</td>
<td>0.1333–101.325</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>650.91</td>
<td>literature summary</td>
<td>115–385</td>
<td>2.33×10(^{-4})–4100</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>24.02°C</td>
<td>102.24</td>
<td>isotenisco pic</td>
<td>–29.65–195.65°C</td>
<td>1.05–4273.89</td>
<td>Benning and McHarness 1940</td>
</tr>
<tr>
<td></td>
<td>293.055 K</td>
<td>88.55</td>
<td>calorimetry static</td>
<td>236–293</td>
<td>6.31–88.55</td>
<td>Osborne et al. 1941</td>
</tr>
<tr>
<td></td>
<td>23.7°C</td>
<td>101.325</td>
<td>literature summary</td>
<td>–84.3–23.7°C</td>
<td>0.1333–101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>106.4</td>
<td>literature summary</td>
<td>162–471</td>
<td>6.26×10(^{-3})–4408</td>
<td>Xiang 2002</td>
</tr>
<tr>
<td>Fluoroethane</td>
<td>25.65°C</td>
<td>932</td>
<td>manometer</td>
<td>25.65–102.16°C</td>
<td>932–5028</td>
<td>Booth and Swinehart 1935</td>
</tr>
<tr>
<td></td>
<td>295.82 K</td>
<td>865.9</td>
<td>static</td>
<td>–103.6––37.1°C</td>
<td>1.33–101</td>
<td>Grosse et al. 1940</td>
</tr>
<tr>
<td></td>
<td>20°C</td>
<td>833.3</td>
<td>static</td>
<td>228–322</td>
<td>70–1699</td>
<td>Vidalurri 1975</td>
</tr>
<tr>
<td></td>
<td>290.76</td>
<td>22</td>
<td>mercury manometer</td>
<td>234–291</td>
<td>0.858–22</td>
<td>Li and Pitzer 1956</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>596</td>
<td>isochoric</td>
<td>239–368</td>
<td>59–3334</td>
<td>Zhao et al. 1992</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>597</td>
<td>strain gauge</td>
<td>281–335</td>
<td>352–1550</td>
<td>Defibaugh and Morrison 1996</td>
</tr>
<tr>
<td></td>
<td>299.995 K</td>
<td>1331</td>
<td>mercury manometer</td>
<td>174–226</td>
<td>3.49–101.01</td>
<td>Russell et al. 1944</td>
</tr>
<tr>
<td></td>
<td>298.22</td>
<td>1265.1</td>
<td>manometer/densimeter</td>
<td>278–340</td>
<td>769–3337</td>
<td>Widiatmo et al. 1994</td>
</tr>
<tr>
<td></td>
<td>300 K</td>
<td>1327.0</td>
<td>isochoric</td>
<td>244–345</td>
<td>226–3717</td>
<td>Giuliani et al. 1995b</td>
</tr>
<tr>
<td></td>
<td>279.484 K</td>
<td>751.294</td>
<td>ebulliometry</td>
<td>236–279</td>
<td>160–751</td>
<td>Zhang et al. 1995a</td>
</tr>
<tr>
<td></td>
<td>298.165 K</td>
<td>1262.0</td>
<td>PVT apparatus</td>
<td>279–343</td>
<td>744–3556</td>
<td>Weber and Defibaugh 1996b</td>
</tr>
<tr>
<td></td>
<td>293.149 K</td>
<td>1104.8</td>
<td>VLE</td>
<td>263–346</td>
<td>447–3763</td>
<td>Weber and Defibaugh 1996b</td>
</tr>
<tr>
<td></td>
<td>283.11</td>
<td>834.8</td>
<td>VLE</td>
<td>3.49–101.01</td>
<td>769–3337</td>
<td>Widiatmo et al. 1994</td>
</tr>
<tr>
<td></td>
<td>298.16</td>
<td>1260.7</td>
<td>VLE</td>
<td>226–3717</td>
<td>769–3337</td>
<td>Widiatmo et al. 1994</td>
</tr>
<tr>
<td></td>
<td>313.21</td>
<td>1832.5</td>
<td>VLE</td>
<td>295–342</td>
<td>164–3474</td>
<td>Widiatmo et al. 1994</td>
</tr>
<tr>
<td></td>
<td>300 K</td>
<td>1325.3</td>
<td>isochoric</td>
<td>236–279</td>
<td>160–751</td>
<td>Zhang et al. 1995a</td>
</tr>
<tr>
<td></td>
<td>298.16</td>
<td>1262.62</td>
<td>Burnett apparatus</td>
<td>251–343</td>
<td>292–3554</td>
<td>Duan et al. 2004</td>
</tr>
<tr>
<td>1,1,2,2-Tetrafluoroethane</td>
<td>299.994 K</td>
<td>546</td>
<td>Burnett apparatus</td>
<td>300–345</td>
<td>1325–3748</td>
<td>Widiatmo et al. 2001</td>
</tr>
<tr>
<td>1,1,1,2-Tetrafluoroethane</td>
<td>299.976 K</td>
<td>699</td>
<td>VLE</td>
<td>280–350</td>
<td>38–2459</td>
<td>Maezawa et al. 1990</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>Property</td>
<td>Reference</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------</td>
<td>----------</td>
<td>-----------</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>297.15 K</td>
<td>645.53</td>
<td>Zhu et al. 1992</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.21 K</td>
<td>666.7</td>
<td>Giuliani et al. 1995a</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.13 K</td>
<td>666</td>
<td>Takagi 1996a</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.66 K</td>
<td>580</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>303.68 K</td>
<td>780.9</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>283.62 K</td>
<td>420.7</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.14 K</td>
<td>571.5</td>
<td>Fujiwara et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.15 K</td>
<td>571.3</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>303.15 K</td>
<td>769.4</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>313.15 K</td>
<td>1014.6</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.21 K</td>
<td>666.7</td>
<td>Giuliani et al. 1995a</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.13 K</td>
<td>666</td>
<td>Takagi 1996a</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.66 K</td>
<td>580</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>303.68 K</td>
<td>780.9</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>283.62 K</td>
<td>420.7</td>
<td>Bobbo et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.14 K</td>
<td>571.5</td>
<td>Fujiwara et al. 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293.15 K</td>
<td>571.3</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>303.15 K</td>
<td>769.4</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>313.15 K</td>
<td>1014.6</td>
<td>Bobbo et al. 2001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Pentafluoroethane**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Property</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>284.714 K</td>
<td>951.5741</td>
<td>Wilson et al. 1992</td>
</tr>
<tr>
<td>299.985 K</td>
<td>1444</td>
<td>Weber and Silva 1994</td>
</tr>
<tr>
<td>300 K</td>
<td>1446.6</td>
<td>Ye et al. 1995</td>
</tr>
<tr>
<td>298.21 K</td>
<td>1380</td>
<td>Takagi 1996b</td>
</tr>
<tr>
<td>299.998 K</td>
<td>1447.57</td>
<td>Duarte-Garza et al. 1997b</td>
</tr>
<tr>
<td>303.19 K</td>
<td>1568.5</td>
<td>Bobbo et al. 1999</td>
</tr>
<tr>
<td>323.26 K</td>
<td>2539.3</td>
<td>Bobbo et al. 1999</td>
</tr>
<tr>
<td>308.15 K</td>
<td>1778.8</td>
<td>Horstmann et al. 2004</td>
</tr>
</tbody>
</table>

**Hexafluoroethane**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Property</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>291.2 K</td>
<td>2902.1</td>
<td>Pace and Aston 1948</td>
</tr>
<tr>
<td>284.688 K</td>
<td>218.216</td>
<td>Silva and Weber 1993</td>
</tr>
<tr>
<td>286.098 K</td>
<td>258.829</td>
<td>Weber and Silva 1994</td>
</tr>
<tr>
<td>299.795 K</td>
<td>83.43</td>
<td>Aston et al. 1955</td>
</tr>
<tr>
<td>308.26 K</td>
<td>131</td>
<td>Mears et al. 1966</td>
</tr>
<tr>
<td>299.988 K</td>
<td>67</td>
<td>Duarte-Garza et al. 1997a</td>
</tr>
<tr>
<td>293.143 K</td>
<td>76.6</td>
<td>Maezawa et al. 1991b</td>
</tr>
<tr>
<td>299.950 K</td>
<td>97.45</td>
<td>Weber 1992</td>
</tr>
</tbody>
</table>

**1,1-Dichloro-1-fluoroethane**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Property</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 K</td>
<td>84.20</td>
<td>Duarte-Garza et al. 1997a</td>
</tr>
<tr>
<td>299.968 K</td>
<td>86</td>
<td>Maezawa et al. 1991b</td>
</tr>
<tr>
<td>299.975 K</td>
<td>83.43</td>
<td>Weber 1992</td>
</tr>
</tbody>
</table>

**1,1-Dichlorotrifluoroethane**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Property</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>289.988 K</td>
<td>67</td>
<td>Maezawa et al. 1990</td>
</tr>
<tr>
<td>308.26 K</td>
<td>131</td>
<td>Piao et al. 1991</td>
</tr>
<tr>
<td>293.143 K</td>
<td>76.6</td>
<td>Oguchi et al. 1992</td>
</tr>
</tbody>
</table>

**1,2-Dichloro-1,1,2,2-tetrafluoroethane**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Property</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.2 K</td>
<td>48.143</td>
<td>Stull 1947</td>
</tr>
<tr>
<td>20.19°C</td>
<td>36.64</td>
<td>Hiraoka and Hildebrand 1963</td>
</tr>
<tr>
<td>30.2°C</td>
<td>53.29</td>
<td>Stull 1947</td>
</tr>
<tr>
<td>Compound</td>
<td>Temp. °C or K</td>
<td>P or kPa</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
<td>----------</td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloro-1,2-difluoroethane</td>
<td>298.2 K</td>
<td>48.476</td>
</tr>
<tr>
<td></td>
<td>20°C</td>
<td>6.106</td>
</tr>
<tr>
<td></td>
<td>19.8°C</td>
<td>5.333</td>
</tr>
<tr>
<td>2-Fluoropropane</td>
<td>30°C</td>
<td>407</td>
</tr>
<tr>
<td></td>
<td>50°C</td>
<td>700</td>
</tr>
<tr>
<td>1,1,2,2,3-Pentafluoropropane</td>
<td>298.98 K</td>
<td>100.7</td>
</tr>
<tr>
<td>1,1,1,3,3-Pentafluoropropane</td>
<td>298.21 K</td>
<td>149.04</td>
</tr>
<tr>
<td>1,1,1,2,3,3-Hexafluoropropane</td>
<td>30°C</td>
<td>535.05</td>
</tr>
<tr>
<td></td>
<td>292.955 K</td>
<td>397.36</td>
</tr>
<tr>
<td>1,1,1,2,3,3-Hexafluoropropane</td>
<td>300 K</td>
<td>219.6</td>
</tr>
<tr>
<td></td>
<td>283.12 K</td>
<td>118.6</td>
</tr>
<tr>
<td></td>
<td>298.16 K</td>
<td>205.8</td>
</tr>
<tr>
<td></td>
<td>313.21 K</td>
<td>340.4</td>
</tr>
<tr>
<td></td>
<td>283.12 K</td>
<td>118.4</td>
</tr>
<tr>
<td></td>
<td>298.17 K</td>
<td>207.0</td>
</tr>
<tr>
<td></td>
<td>313.22 K</td>
<td>338.5</td>
</tr>
<tr>
<td></td>
<td>298.41 K</td>
<td>208.1</td>
</tr>
<tr>
<td>1,1,1,3,3,3-Hexafluoropropane</td>
<td>299.15 K</td>
<td>281.15</td>
</tr>
<tr>
<td></td>
<td>283.62 K</td>
<td>162.6</td>
</tr>
<tr>
<td></td>
<td>303.68 K</td>
<td>325.8</td>
</tr>
<tr>
<td></td>
<td>303.2 K</td>
<td>322.2</td>
</tr>
<tr>
<td></td>
<td>323.26 K</td>
<td>584.2</td>
</tr>
<tr>
<td></td>
<td>323.26 K</td>
<td>585.7</td>
</tr>
<tr>
<td></td>
<td>298.27 K</td>
<td>272.5</td>
</tr>
<tr>
<td></td>
<td>283.13 K</td>
<td>160.0</td>
</tr>
<tr>
<td></td>
<td>303.19 K</td>
<td>322.3</td>
</tr>
<tr>
<td>Compound</td>
<td>Temperature</td>
<td>Pressure</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>-------------</td>
<td>-----------</td>
</tr>
<tr>
<td>1,1,1,2,3,3,3-Heptafluoropropane</td>
<td>299.06 K</td>
<td>467.35</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Octafluoropropane</td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Trichlorotrifluoropropene</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>1-Chloro-2,2,2-trifluoropropane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluorobutane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluorocyclobutane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluoropentane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluorocyclopentane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluoro-2-methylcyclopentane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluoro-3-methylcyclopentane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluorocyclohexane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
<tr>
<td>Perfluorohexane</td>
<td>20°C</td>
<td>232.033</td>
</tr>
<tr>
<td></td>
<td>29.17°C</td>
<td>9.69 atm</td>
</tr>
<tr>
<td></td>
<td>298.152 K</td>
<td>441.61</td>
</tr>
<tr>
<td></td>
<td>295.27 K</td>
<td>416.1</td>
</tr>
<tr>
<td></td>
<td>297.22 K</td>
<td>441.61</td>
</tr>
</tbody>
</table>
| (Continued)
### TABLE 5.1.5.3 (Continued)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Temp. °C or K</th>
<th>P* kPa</th>
<th>Method*</th>
<th>Temp. Range** °C or K</th>
<th>Pressure Range kPa</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluoroalkenes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorotrifluoroethene</td>
<td>21.9°C</td>
<td>577.55</td>
<td>manometer</td>
<td>–131 – –65°C</td>
<td>1–177</td>
<td>Furukava et al. 1953*</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>195–250 K</td>
<td>6–123</td>
<td>Booth et al. 1933</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>literature summary</td>
<td>21.9–107°C</td>
<td>577.55–3951.68</td>
<td>Booth and Swinehart 1935</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>calorimetry static</td>
<td>–116 – –27.9°C</td>
<td>0.1333–101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>–67 – –11 °C</td>
<td>13–205</td>
<td>Oliver et al. 1951</td>
</tr>
<tr>
<td>1,2-Dichloro-1,2-difluoroethene</td>
<td>295 K</td>
<td>105.8</td>
<td>manometer</td>
<td>240–295 K</td>
<td>8–106</td>
<td>Booth et al. 1933</td>
</tr>
<tr>
<td></td>
<td>20.9°C</td>
<td>101.325</td>
<td>literature summary</td>
<td>–82.0–20.9°C</td>
<td>0.1333–101.325</td>
<td>Stull 1947</td>
</tr>
<tr>
<td>1,1-Dichloro-2,2-difluoroethene</td>
<td>295 K</td>
<td>105.8</td>
<td>manometer</td>
<td>240–295 K</td>
<td>8–106</td>
<td>Booth et al. 1933</td>
</tr>
<tr>
<td>Hexafluoropropene</td>
<td>19.75°C</td>
<td>652.7</td>
<td></td>
<td>–41–20°C</td>
<td>62–653</td>
<td>Whipple 1952</td>
</tr>
</tbody>
</table>

* VLE – vapor-liquid equilibrium.
** For temperature dependence equation, see reference.
* Boublik et al. 1984.
## Table 5.1.5.4
Henry's law constants and octanol-water partition coefficients for fluoroalkanes and fluoroalkenes

<table>
<thead>
<tr>
<th>Compound</th>
<th>Henry's law constant</th>
<th>Temp °C</th>
<th>Method/temp. range</th>
<th>Reference</th>
<th>K_{OW}</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluoroalkanes</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoromethane</td>
<td>1418</td>
<td>25</td>
<td>calculated</td>
<td>Yaws et al. 1991</td>
<td>0.51</td>
<td>Sangster 1993</td>
</tr>
<tr>
<td></td>
<td>1948</td>
<td>20</td>
<td></td>
<td>Glew &amp; Moelwyn-Hughes 1953</td>
<td>0.51</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td></td>
<td>1717</td>
<td>25</td>
<td>calculated C_{A}/C_{W}</td>
<td>Hine &amp; Mookerjee 1975</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1742</td>
<td>20T</td>
<td></td>
<td>Staudinger &amp; Roberts 2001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Difluoromethane</td>
<td>1160</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>0.20</td>
<td>Sangster 1993,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Trifluoromethane</td>
<td>5907</td>
<td>25</td>
<td>gas stripping-GC</td>
<td>Warner et al. 1987</td>
<td>0.64</td>
<td>Hansch &amp; Leo 1985</td>
</tr>
<tr>
<td></td>
<td>9211</td>
<td>25</td>
<td></td>
<td>Hine &amp; Mookerjee 1975</td>
<td>0.64</td>
<td>Sangster 1993</td>
</tr>
<tr>
<td></td>
<td>7794</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>0.64</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td></td>
<td>9626</td>
<td>25</td>
<td>calculated-P/C</td>
<td>Howard 1993</td>
<td>0.64</td>
<td>Howard 1993,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Tetrafluoromethane</td>
<td>539961</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>1.18</td>
<td>Sangster 1993,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Chlorofluoromethane</td>
<td>654.4</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>1.55</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Dichlorofluoromethane</td>
<td>529.1</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>1.08</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Chlorodifluoromethane</td>
<td>3058</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>1.08</td>
<td>Howard 1993</td>
</tr>
<tr>
<td>Chlorotrifluoromethane</td>
<td>113889</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>1.65</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>28704</td>
<td>19.93</td>
<td>0–40°C</td>
<td>Warner &amp; Weiss 1985</td>
<td>2.16</td>
<td>Hansch et al. 1996</td>
</tr>
<tr>
<td></td>
<td>39557</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>2.16</td>
<td>Howard 1997</td>
</tr>
<tr>
<td></td>
<td>27976</td>
<td>25</td>
<td></td>
<td>Howard 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>26810</td>
<td>20T</td>
<td></td>
<td>Staudinger &amp; Roberts 2001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>7925</td>
<td>19.93</td>
<td>0–40°C</td>
<td>Warner &amp; Weiss 1985</td>
<td>2.53</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td></td>
<td>10234</td>
<td>25T</td>
<td></td>
<td>Ashworth et al. 1988</td>
<td>2.53</td>
<td>Howard 1990</td>
</tr>
<tr>
<td></td>
<td>9827</td>
<td>25</td>
<td></td>
<td>Howard 1990</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>12341</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7824</td>
<td>20T</td>
<td></td>
<td>Staudinger &amp; Roberts 2001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoroethane</td>
<td>2253</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>0.75</td>
<td>Hansch et al. 1995</td>
</tr>
<tr>
<td>1,1-Difluoroethane</td>
<td>2672</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td>0.75</td>
<td>Sangster 1993</td>
</tr>
<tr>
<td></td>
<td>2203</td>
<td>25</td>
<td></td>
<td>Hine &amp; Mookerjee 1975</td>
<td>0.75</td>
<td>Howard 1993</td>
</tr>
<tr>
<td></td>
<td>2061</td>
<td>20T</td>
<td></td>
<td>Howard 1993</td>
<td>0.75</td>
<td>Howard 1993</td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th>Compound</th>
<th>Henry’s law constant Pa•m³/mol</th>
<th>Temp. °C</th>
<th>Method/temp. range</th>
<th>Reference</th>
<th>K_{OW}</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,1,2-Trifluoroethane</td>
<td>1876</td>
<td>25</td>
<td></td>
<td>Zheng et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>32323</td>
<td>25T</td>
<td>EPICS-GC</td>
<td>Ashworth et al. 1988</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,1,2-Tetrafluoroethane</td>
<td>5629</td>
<td>25T</td>
<td></td>
<td>Zheng et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexafluoroethane</td>
<td>1715432</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1652940</td>
<td>25T</td>
<td></td>
<td>Bonifacio et al. 2001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,1-difluoroethane</td>
<td>24217</td>
<td>25</td>
<td>calc-bond contribution</td>
<td>Howard 1990</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,2,2,2-tetrafluoroethane</td>
<td>54716</td>
<td>25</td>
<td></td>
<td>Howard 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Chloropentafluoroethane</td>
<td>261418</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>309041</td>
<td>25</td>
<td></td>
<td>Howard 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloro-1-fluoroethane</td>
<td>2442</td>
<td>25</td>
<td></td>
<td>Howard 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2-Dichlorotetrafluoroethane</td>
<td>122502</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Dichlorotetrafluoroethane</td>
<td>49132</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,2-Trichloro-1,2,2-trifluoroethane</td>
<td>53297</td>
<td>25</td>
<td>calculated-P/C</td>
<td>Howard 1990</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Difluorotetrachloroethane</td>
<td>171239</td>
<td>25</td>
<td></td>
<td>Howard 1993</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2-Difluoro-1,1,2,2-tetrafluoroethane</td>
<td>283710</td>
<td>25</td>
<td>calculated-P/C</td>
<td>Howard 1990</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloro-1,2-difluoroethane</td>
<td>9869</td>
<td>25</td>
<td>calculated-C_{A}/C_{W}</td>
<td>Hine &amp; Mookerjee 1975</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Fluoropropane</td>
<td>1627</td>
<td>14</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-Fluoropropane</td>
<td>1713</td>
<td>15</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Perfluorocyclobutane</td>
<td>391925</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoroalkenes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,1-Difluoroethene</td>
<td>39344</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tetrafluoroethene</td>
<td>61981</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorotrifluoroethene</td>
<td>63328</td>
<td>25</td>
<td></td>
<td>Yaws et al. 1991</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexafluoropropene</td>
<td>349397</td>
<td>25</td>
<td></td>
<td>Wilhelm et al. 1977</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### TABLE 5.1.5.5
Atmospheric fate rates for fluoroalkanes

<table>
<thead>
<tr>
<th>Compound</th>
<th>T/K</th>
<th>k&lt;sub&gt;OH&lt;/sub&gt;*/(cm&lt;sup&gt;3&lt;/sup&gt; molecule&lt;sup&gt;-1&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>Temp. range**</th>
<th>Lifetime, τ</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluoroalkanes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluoromethane</td>
<td>296</td>
<td>16×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.68×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>294–480 K</td>
<td>2–4.1 yr</td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Difluoromethane</td>
<td>296</td>
<td>7.8×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>7.2×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td>293–425 K</td>
<td>2–4.1 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.09×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>250–492 K</td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.13×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>222–381 K</td>
<td>7.1–7.7 yr</td>
<td>Talukdar et al. 1991</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>Trifluoromethane</td>
<td>296</td>
<td>0.2×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>2.4×10&lt;sup&gt;-16&lt;/sup&gt;</td>
<td>387–1445</td>
<td>4–7.3 yr</td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Tetrafluoromethane</td>
<td>298</td>
<td>&lt;4×10&lt;sup&gt;-16&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Chlorofluoromethane</td>
<td>296</td>
<td>37×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>4.41×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>245–486 K</td>
<td>4–7.3 yr</td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Dichlorofluoromethane</td>
<td>296</td>
<td>26×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>3.9×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>293–425 K</td>
<td></td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>3.03×10&lt;sup&gt;-14&lt;/sup&gt;</td>
<td>241–483 K</td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Chlorodifluoromethane</td>
<td>296</td>
<td>3.4×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>4.1×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td>293–425 K</td>
<td></td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>4.68×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td>250–482 K</td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Chlorotrifluoromethane</td>
<td>296</td>
<td>&lt;0.7×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td>17.2 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>&lt;7×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>296</td>
<td>&lt;1.0×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td>105 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>296</td>
<td>&lt;0.4×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>293</td>
<td>&lt;10&lt;sup&gt;-16&lt;/sup&gt;</td>
<td></td>
<td>&gt;330 yr</td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>296</td>
<td>&lt;1.0×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Atkinson 1975</td>
</tr>
<tr>
<td></td>
<td>296</td>
<td>&lt;0.5×10&lt;sup&gt;-15&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Howard &amp; Evenson 1976a</td>
</tr>
<tr>
<td></td>
<td>293</td>
<td>&lt;10&lt;sup&gt;-17&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>&lt;1.0×10&lt;sup&gt;-17&lt;/sup&gt;</td>
<td></td>
<td></td>
<td>Atkinson 1989</td>
</tr>
</tbody>
</table>
### TABLE 5.1.5.5 (Continued)

<table>
<thead>
<tr>
<th>Compound</th>
<th>T/K</th>
<th>$k_{\text{OH}}$/(cm$^3$ molecule$^{-1}$ s$^{-1}$)</th>
<th>Temp. range**</th>
<th>Lifetime, $\tau$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluoroethane</td>
<td></td>
<td></td>
<td></td>
<td>60 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>182–635 yr</td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>1,1-Difluoroethane</td>
<td>298</td>
<td>5.1x10$^{-14}$</td>
<td>293–425 K</td>
<td>0.2–1 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>295</td>
<td>3.4x10$^{-14}$</td>
<td>293–425 K</td>
<td>1.5 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>303</td>
<td>5.6x10$^{-14}$</td>
<td>230–423 K</td>
<td>1.5 yr</td>
<td>Li et al. 1990</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>4.2x10$^{-14}$</td>
<td>243–400 K</td>
<td>1–1.68 yr</td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>1,2-Difluoroethane</td>
<td></td>
<td></td>
<td></td>
<td>0.58–0.8 yr</td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>1,1,1-Trifluoroethane</td>
<td>298</td>
<td>1.5x10$^{-15}$</td>
<td>293–425 K</td>
<td>72–74 yr</td>
<td>Atkinson 1989</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.35x10$^{-15}$</td>
<td>223–374 K</td>
<td>6.3 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>303</td>
<td>6.9x10$^{-15}$</td>
<td>231–423 K</td>
<td>20–45 yr</td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>1,1,2-Trifluoroethane</td>
<td>298</td>
<td>4.9x10$^{-14}$</td>
<td>293–425 K</td>
<td>1–3.8 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td>1,1,2,2-Tetrafluoroethane</td>
<td>298</td>
<td>6.9x10$^{-15}$</td>
<td>293–425 K</td>
<td>1–3.8 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>8.54x10$^{-15}$</td>
<td>249–473 K</td>
<td>1–3.8 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td>1,1,1,2-Tetrafluoroethane</td>
<td>298</td>
<td>6.9x10$^{-15}$</td>
<td>293–425 K</td>
<td>2–12.3 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>301</td>
<td>6.9x10$^{-15}$</td>
<td>231–423 K</td>
<td>10.7 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>5.18x10$^{-15}$</td>
<td>243–400 K</td>
<td>14.4 yr</td>
<td>Li et al. 1990</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>13.1–15.5 yr</td>
<td>Franklin 1993</td>
</tr>
<tr>
<td>Pentafluoroethane</td>
<td>298</td>
<td>5.0x10$^{-15}$</td>
<td>293–425 K</td>
<td>22.1 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>303</td>
<td>2.9x10$^{-15}$</td>
<td>223–375 K</td>
<td>47–48 yr</td>
<td>Talukdar et al. 1991</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.9x10$^{-15}$</td>
<td>220–364 K</td>
<td>17–28.1 yr</td>
<td>Cooper et al. 1992</td>
</tr>
<tr>
<td>1-Chloro-1,1-difluoroethane</td>
<td>298</td>
<td>6.74x10$^{-15}$</td>
<td>293–425 K</td>
<td>15.4 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>3.58x10$^{-15}$</td>
<td>273–375 K</td>
<td>15.4 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>303</td>
<td>3.7x10$^{-15}$</td>
<td>231–423 K</td>
<td>15.4 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>4.02x10$^{-15}$</td>
<td>243–400 K</td>
<td>15.4 yr</td>
<td>Brown et al. 1990</td>
</tr>
<tr>
<td>1-Chloro-1,1,2-trifluoroethane</td>
<td>298</td>
<td>1.5x10$^{-14}$</td>
<td>293–425 K</td>
<td>1.5 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td></td>
<td>298</td>
<td>1.61x10$^{-14}$</td>
<td>263–373 K</td>
<td>1.5 yr</td>
<td>Clyne et al. 1978</td>
</tr>
<tr>
<td>Substance</td>
<td>k&lt;sub&gt;OH&lt;/sub&gt;</td>
<td>T&lt;sub&gt;min&lt;/sub&gt;–T&lt;sub&gt;max&lt;/sub&gt; K</td>
<td>t&lt;sub&gt;1/2&lt;/sub&gt; yr</td>
<td>Reference</td>
<td></td>
</tr>
<tr>
<td>-----------------------------------------------</td>
<td>----------------</td>
<td>----------------------------------</td>
<td>------------------</td>
<td>-------------------</td>
<td></td>
</tr>
<tr>
<td>1-Chloro-1,2,2,2-tetrafluoroethane</td>
<td>1.02×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>250–375 K</td>
<td></td>
<td>Atkinson 1989</td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloro-1-fluoroethane</td>
<td>7.1×10&lt;sup&gt;−15&lt;/sup&gt;</td>
<td>243–400 K</td>
<td>6.7 yr</td>
<td>Liu et al. 1990</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.61×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>238–426 K</td>
<td>4.3 yr</td>
<td>Brown et al. 1990</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.92×10&lt;sup&gt;−15&lt;/sup&gt;</td>
<td>233–393 K</td>
<td>13–14 yr</td>
<td>Talukdar et al. 1991</td>
<td></td>
</tr>
<tr>
<td>1,2-Dichloro-1,1-difluoroethane</td>
<td>2.61×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>249–473 K</td>
<td></td>
<td>Atkinson 1989</td>
<td></td>
</tr>
<tr>
<td>1,1-Dichlorotrifluoroethane</td>
<td>4.2×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>293–425 K</td>
<td></td>
<td>Clyne et al. 1978</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.34×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>245–375 K</td>
<td></td>
<td>Atkinson 1989</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.9×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>232–425 K</td>
<td>1.0 yr</td>
<td>Brown et al. 1990</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.52×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>270–400 K</td>
<td>1.4 yr</td>
<td>Liu et al. 1990</td>
<td></td>
</tr>
<tr>
<td>1,1,2,2,3-Pentafluoropropane</td>
<td>2×10&lt;sup&gt;−14&lt;/sup&gt;, 4×10&lt;sup&gt;−14&lt;/sup&gt;</td>
<td>2, 1.3 yr</td>
<td></td>
<td>Cooper et al. 1993</td>
<td></td>
</tr>
<tr>
<td>1,1,1,2,2-Pentafluoropropane</td>
<td>7×10&lt;sup&gt;−15&lt;/sup&gt;, 8×10&lt;sup&gt;−15&lt;/sup&gt;</td>
<td>7 yr</td>
<td></td>
<td>Cooper et al. 1993</td>
<td></td>
</tr>
<tr>
<td>1,1,1,2,3,3-Hexafluoropropane</td>
<td>4×10&lt;sup&gt;−15&lt;/sup&gt;, 6×10&lt;sup&gt;−15&lt;/sup&gt;</td>
<td>10, 9 yr</td>
<td></td>
<td>Cooper et al. 1993</td>
<td></td>
</tr>
<tr>
<td>1,1,1,3,3,3-Hexafluoropropane</td>
<td>5×10&lt;sup&gt;−16&lt;/sup&gt;, 2×10&lt;sup&gt;−16&lt;/sup&gt;</td>
<td>77, 218 yr</td>
<td></td>
<td>Cooper et al. 1993</td>
<td></td>
</tr>
<tr>
<td>1,1,1,2,3,3,3-Heptafluoropropane</td>
<td>7×10&lt;sup&gt;−16&lt;/sup&gt;</td>
<td>63, 72 yr</td>
<td></td>
<td>Cooper et al. 1993</td>
<td></td>
</tr>
</tbody>
</table>

* k<sub>OH</sub> = second order reaction rate constant with hydroxyl radicals
** For temperature dependence equation, see reference.
## 5.1.5 FLUOROALKANES AND FLUOROALKENES

### TABLE 5.2.1

Summary of physical properties of halogenated hydrocarbons

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p., °C</th>
<th>b.p., °C</th>
<th>Fugacity ratio, F at 23°C*</th>
<th>Molar volume, ( V_m ) cm³/mol</th>
<th>MW/( \rho ) at 20°C</th>
<th>Le Bas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chloroalkanes:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chloromethane (Methyl chloride)</td>
<td>74-87-3</td>
<td>( \text{CH}_3\text{Cl} )</td>
<td>50.488</td>
<td>97.7</td>
<td>24.09</td>
<td>1</td>
<td>54.79</td>
<td>50.5</td>
<td></td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>75-09-2</td>
<td>( \text{CH}_2\text{Cl}_2 )</td>
<td>84.933</td>
<td>97.2</td>
<td>40</td>
<td>1</td>
<td>64.07</td>
<td>71.4</td>
<td></td>
</tr>
<tr>
<td>Trichloromethane (Chloroform)</td>
<td>67-66-3</td>
<td>( \text{CHCl}_3 )</td>
<td>119.378</td>
<td>63.41</td>
<td>61.17</td>
<td>1</td>
<td>79.67</td>
<td>92.3</td>
<td></td>
</tr>
<tr>
<td>Tetrachloromethane (Carbon tetrachloride)</td>
<td>56-23-5</td>
<td>( \text{CCl}_4 )</td>
<td>153.823</td>
<td>22.62</td>
<td>76.8</td>
<td>1</td>
<td>96.50</td>
<td>113.2</td>
<td></td>
</tr>
<tr>
<td>Chloroethane (Ethyl chloride)</td>
<td>75-00-3</td>
<td>( \text{C}_2\text{H}_4\text{Cl} )</td>
<td>64.514</td>
<td>138.4</td>
<td>12.3</td>
<td>1</td>
<td>72.00</td>
<td>72.7</td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloroethane</td>
<td>75-34-3</td>
<td>( \text{C}_2\text{H}_4\text{Cl}_2 )</td>
<td>98.959</td>
<td>96.9</td>
<td>57.3</td>
<td>1</td>
<td>84.18</td>
<td>93.6</td>
<td></td>
</tr>
<tr>
<td>1,2-Dichloroethane</td>
<td>107-06-2</td>
<td>( \text{C}_2\text{H}_4\text{Cl}_2 )</td>
<td>98.959</td>
<td>35.7</td>
<td>85.3</td>
<td>1</td>
<td>79.04</td>
<td>93.6</td>
<td></td>
</tr>
<tr>
<td>1,1,1-Trichloroethane</td>
<td>71-55-6</td>
<td>( \text{C}_2\text{H}_3\text{Cl}_3 )</td>
<td>133.404</td>
<td>30.01</td>
<td>74.09</td>
<td>1</td>
<td>99.70</td>
<td>114.5</td>
<td></td>
</tr>
<tr>
<td>1,1,2-Trichloroethane</td>
<td>79-00-5</td>
<td>( \text{C}_2\text{H}_3\text{Cl}_3 )</td>
<td>133.404</td>
<td>36.3</td>
<td>113.8</td>
<td>1</td>
<td>92.69</td>
<td>114.5</td>
<td></td>
</tr>
<tr>
<td>1,1,1,2-Tetrachloroethane</td>
<td>630-20-6</td>
<td>( \text{C}_2\text{H}_2\text{Cl}_4 )</td>
<td>167.849</td>
<td>–70.2</td>
<td>130.2</td>
<td>1</td>
<td>108.95</td>
<td>135.4</td>
<td></td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloroethane</td>
<td>79-34-5</td>
<td>( \text{C}_2\text{H}_2\text{Cl}_4 )</td>
<td>167.849</td>
<td>–42.4</td>
<td>145.2</td>
<td>1</td>
<td>105.27</td>
<td>135.4</td>
<td></td>
</tr>
<tr>
<td>Pentachloroethane</td>
<td>76-01-7</td>
<td>( \text{C}_2\text{H}_2\text{Cl}_5 )</td>
<td>202.294</td>
<td>–28.78</td>
<td>162.0</td>
<td>1</td>
<td>120.36</td>
<td>156.3</td>
<td></td>
</tr>
<tr>
<td>Hexachloroethane</td>
<td>67-72-1</td>
<td>( \text{C}_2\text{H}_2\text{Cl}_6 )</td>
<td>236.739</td>
<td></td>
<td></td>
<td>1</td>
<td>113.22</td>
<td>177.2</td>
<td></td>
</tr>
<tr>
<td>1-Chloropropane (n-Propyl chloride)</td>
<td>540-54-5</td>
<td>( \text{C}_3\text{H}_7\text{Cl} )</td>
<td>78.541</td>
<td>–122.9</td>
<td>46.5</td>
<td>1</td>
<td>88.26</td>
<td>94.9</td>
<td></td>
</tr>
<tr>
<td>2-Chloropropane</td>
<td>75-29-6</td>
<td>( \text{C}_3\text{H}_7\text{Cl} )</td>
<td>78.541</td>
<td>–117.18</td>
<td>35.7</td>
<td>1</td>
<td>91.15</td>
<td>94.9</td>
<td></td>
</tr>
<tr>
<td>1,2-Dichloropropane</td>
<td>78-87-5</td>
<td>( \text{C}_3\text{H}_6\text{Cl}_2 )</td>
<td>112.986</td>
<td>–100.53</td>
<td>96.4</td>
<td>1</td>
<td>97.74</td>
<td>115.8</td>
<td></td>
</tr>
<tr>
<td>1,2,3-Trichloropropane</td>
<td>96-18-4</td>
<td>( \text{C}_3\text{H}_6\text{Cl}_3 )</td>
<td>147.431</td>
<td>–14.7</td>
<td>157</td>
<td>1</td>
<td>106.59</td>
<td>136.7</td>
<td></td>
</tr>
<tr>
<td>1-Chlorobutane (n-Butyl chloride)</td>
<td>109-69-3</td>
<td>( \text{C}_4\text{H}_9\text{Cl} )</td>
<td>92.567</td>
<td>–123.1</td>
<td>78.4</td>
<td>1</td>
<td>104.51</td>
<td>117.1</td>
<td></td>
</tr>
<tr>
<td>2-Chlorobutane</td>
<td>78-86-4</td>
<td>( \text{C}_4\text{H}_9\text{Cl} )</td>
<td>92.567</td>
<td>–131.3</td>
<td>68.2</td>
<td>1</td>
<td>106.01</td>
<td>117.1</td>
<td></td>
</tr>
<tr>
<td>1-Chloropentane (n-Amyl chloride)</td>
<td>543-59-6</td>
<td>( \text{C}<em>5\text{H}</em>{11}\text{Cl} )</td>
<td>106.594</td>
<td>–99.0</td>
<td>108.4</td>
<td>1</td>
<td>120.85</td>
<td>139.3</td>
<td></td>
</tr>
<tr>
<td>1-Chlorohexane</td>
<td>544-10-5</td>
<td>( \text{C}<em>6\text{H}</em>{13}\text{Cl} )</td>
<td>120.620</td>
<td>–94.0</td>
<td>135.1</td>
<td>1</td>
<td>137.30</td>
<td>161.5</td>
<td></td>
</tr>
<tr>
<td>1-Chloroheptane</td>
<td>629–06-1</td>
<td>( \text{C}<em>7\text{H}</em>{15}\text{Cl} )</td>
<td>134.647</td>
<td>–69.5</td>
<td>160.4</td>
<td>1</td>
<td>153.74</td>
<td>183.7</td>
<td></td>
</tr>
<tr>
<td>1-Chlorooctane</td>
<td>111–85-3</td>
<td>( \text{C}<em>8\text{H}</em>{17}\text{Cl} )</td>
<td>148.674</td>
<td>–57.8</td>
<td>183.5</td>
<td>1</td>
<td>170.15</td>
<td>205.9</td>
<td></td>
</tr>
<tr>
<td>1-Chlrononane</td>
<td>2473–01-0</td>
<td>( \text{C}<em>9\text{H}</em>{19}\text{Cl} )</td>
<td>162.700</td>
<td>–39.4</td>
<td>205.2</td>
<td>1</td>
<td>206.31</td>
<td>228.1</td>
<td></td>
</tr>
<tr>
<td>1-Chlorodecane</td>
<td>1002–69-3</td>
<td>( \text{C}<em>{10}\text{H}</em>{21}\text{Cl} )</td>
<td>176.727</td>
<td>–31.3</td>
<td>225.9</td>
<td>1</td>
<td>203.02</td>
<td>250.3</td>
<td></td>
</tr>
</tbody>
</table>
### Chloroalkenes:

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS</th>
<th>Molecular Formula</th>
<th>Boiling Point (°C)</th>
<th>Flash Point (°C)</th>
<th>Density (g/cm³)</th>
<th>Water Solubility</th>
<th>Octanol/Water Partition Coefficient</th>
<th>Vapour Pressure (mmHg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chloroethene (Vinyl chloride)</td>
<td>75-01-4</td>
<td>C₂H₃Cl</td>
<td>−153.84</td>
<td>−13.8</td>
<td>1</td>
<td>68.63</td>
<td>65.3</td>
<td></td>
</tr>
<tr>
<td>1,1-Dichloroethene</td>
<td>75-35-4</td>
<td>C₂H₂Cl₂</td>
<td>−122.56</td>
<td>31.6</td>
<td>1</td>
<td>79.91</td>
<td>86.2</td>
<td></td>
</tr>
<tr>
<td>cis-1,2-Dichloroethene</td>
<td>156-59-2</td>
<td>C₂H₂Cl₂</td>
<td>−80.0</td>
<td>60.1</td>
<td>1</td>
<td>75.52</td>
<td>86.2</td>
<td></td>
</tr>
<tr>
<td>trans-1,2-Dichloroethene</td>
<td>156-60-5</td>
<td>C₂H₂Cl₂</td>
<td>−49.8</td>
<td>48.7</td>
<td>1</td>
<td>77.15</td>
<td>86.2</td>
<td></td>
</tr>
<tr>
<td>Trichloroethylene</td>
<td>79-01-6</td>
<td>C₃HCl₃</td>
<td>−84.7</td>
<td>87.21</td>
<td>1</td>
<td>89.73</td>
<td>107.1</td>
<td></td>
</tr>
<tr>
<td>Tetrachloroethylene</td>
<td>127-18-4</td>
<td>C₄Cl₄</td>
<td>−22.3</td>
<td>121.3</td>
<td>1</td>
<td>120.19</td>
<td>128.0</td>
<td></td>
</tr>
<tr>
<td>cis-1,3-Dichloropropene</td>
<td>10061-01-5</td>
<td>C₃H₂Cl₂</td>
<td>110.970</td>
<td>104.3</td>
<td>1</td>
<td>91.18</td>
<td>108.4</td>
<td></td>
</tr>
<tr>
<td>trans-1,3-Dichloropropene</td>
<td>10061-02-6</td>
<td>C₃H₂Cl₂</td>
<td>110.970</td>
<td>112</td>
<td>1</td>
<td>90.66</td>
<td>108.4</td>
<td></td>
</tr>
<tr>
<td>Chloroprene</td>
<td>126-99-8</td>
<td>C₃H₅Cl</td>
<td>−130</td>
<td>59.4</td>
<td>1</td>
<td>92.39</td>
<td>102.3</td>
<td></td>
</tr>
<tr>
<td>Hexachloro-1,3-butadiene</td>
<td>87-68-3</td>
<td>C₆H₆Cl₃</td>
<td>−21</td>
<td>215</td>
<td>1</td>
<td>155.03</td>
<td>206.8</td>
<td></td>
</tr>
<tr>
<td>Hexachlorocyclopentadiene</td>
<td>77-47-4</td>
<td>C₇H₉Cl₃</td>
<td>−9</td>
<td>239</td>
<td>1</td>
<td>160.27</td>
<td>210.1</td>
<td></td>
</tr>
</tbody>
</table>

### Bromoalkanes and bromoalkenes:

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS</th>
<th>Molecular Formula</th>
<th>Boiling Point (°C)</th>
<th>Flash Point (°C)</th>
<th>Density (g/cm³)</th>
<th>Water Solubility</th>
<th>Octanol/Water Partition Coefficient</th>
<th>Vapour Pressure (mmHg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bromomethane</td>
<td>74-83-9</td>
<td>CH₂Br</td>
<td>−93.68</td>
<td>3.5</td>
<td>1</td>
<td>56.66</td>
<td>52.9</td>
<td></td>
</tr>
<tr>
<td>Dibromomethane</td>
<td>74-95-3</td>
<td>CH₂Br₂</td>
<td>173.835</td>
<td>97</td>
<td>1</td>
<td>69.62</td>
<td>76.2</td>
<td></td>
</tr>
<tr>
<td>Tribromomethane</td>
<td>75-25-2</td>
<td>CHBr₃</td>
<td>252.731</td>
<td>149.1</td>
<td>1</td>
<td>87.42</td>
<td>99.5</td>
<td></td>
</tr>
<tr>
<td>Bromoethane (Ethyl bromide)</td>
<td>74-96-4</td>
<td>C₂H₃Br</td>
<td>−118.6</td>
<td>38.5</td>
<td>1</td>
<td>75.12</td>
<td>75.1</td>
<td></td>
</tr>
<tr>
<td>1,2-Dibromoethane</td>
<td>106-93-4</td>
<td>C₂H₄Br₂</td>
<td>187.861</td>
<td>131.6</td>
<td>1</td>
<td>86.21</td>
<td>98.4</td>
<td></td>
</tr>
<tr>
<td>1-Bromopropane (n-Propyl bromide)</td>
<td>106-94-5</td>
<td>C₃H₆Br</td>
<td>−110.3</td>
<td>71.1</td>
<td>1</td>
<td>90.86</td>
<td>97.3</td>
<td></td>
</tr>
<tr>
<td>1-Bromopropane</td>
<td>75-26-3</td>
<td>C₃H₆Br</td>
<td>−89.0</td>
<td>59.5</td>
<td>1</td>
<td>93.60</td>
<td>97.3</td>
<td></td>
</tr>
<tr>
<td>1,2-Dibromopropane</td>
<td>78-75-1</td>
<td>C₃H₇Br₂</td>
<td>201.888</td>
<td>141.9</td>
<td>1</td>
<td>104.48</td>
<td>120.6</td>
<td></td>
</tr>
<tr>
<td>1-Bromobutane (n-Butyl bromide)</td>
<td>109-65-9</td>
<td>C₄H₈Br</td>
<td>−112.6</td>
<td>101.6</td>
<td>1</td>
<td>107.40</td>
<td>119.5</td>
<td></td>
</tr>
<tr>
<td>1-Bromopentane (n-Amyl bromide)</td>
<td>110–53–2</td>
<td>C₅H₁₀Br</td>
<td>−88.0</td>
<td>129.8</td>
<td>1</td>
<td>123.99</td>
<td>141.7</td>
<td></td>
</tr>
<tr>
<td>1-Bromohexane</td>
<td>111–25–1</td>
<td>C₆H₁₂Br</td>
<td>−83.7</td>
<td>155.3</td>
<td>1</td>
<td>140.56</td>
<td>163.9</td>
<td></td>
</tr>
<tr>
<td>1-Bromohexane</td>
<td>111–25–1</td>
<td>C₆H₁₂Br</td>
<td>−83.7</td>
<td>155.3</td>
<td>1</td>
<td>140.56</td>
<td>163.9</td>
<td></td>
</tr>
<tr>
<td>1-Bromooctane</td>
<td>111–83–1</td>
<td>C₈H₁₆Br</td>
<td>193.123</td>
<td>200.8</td>
<td>1</td>
<td>173.64</td>
<td>208.3</td>
<td></td>
</tr>
<tr>
<td>1-Bromodecane</td>
<td>112–29–8</td>
<td>C₁₀H₂₀Br</td>
<td>221.178</td>
<td>240.6</td>
<td>1</td>
<td>206.67</td>
<td>252.7</td>
<td></td>
</tr>
<tr>
<td>1-Bromododecane</td>
<td>143–15–7</td>
<td>C₁₂H₂₄Br</td>
<td>−9.5</td>
<td>276</td>
<td>1</td>
<td>239.67</td>
<td>297.1</td>
<td></td>
</tr>
<tr>
<td>Bromocyclohexane</td>
<td>108–85–0</td>
<td>C₁₄H₂₄Br</td>
<td>−56.5</td>
<td>166.2</td>
<td>1</td>
<td>122.06</td>
<td>141.5</td>
<td></td>
</tr>
<tr>
<td>Vinyl bromide</td>
<td>593–60–2</td>
<td>C₂H₅Br</td>
<td>−139.54</td>
<td>15.8</td>
<td>1</td>
<td>71.62</td>
<td>67.7</td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Iodoalkanes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iodomethane (Methyl iodide)</td>
<td>74-88-4</td>
<td>CH$_3$I</td>
<td>141.939</td>
<td>–66.4</td>
<td>42.43</td>
<td>1</td>
<td>62.28</td>
</tr>
<tr>
<td>Iodoethane (Ethyl iodide)</td>
<td>75-03-6</td>
<td>C$_2$H$_5$I</td>
<td>155.965</td>
<td>–111.1</td>
<td>72.3</td>
<td>1</td>
<td>80.57</td>
</tr>
<tr>
<td>1-Iodopropane ($n$-Propyl iodide)</td>
<td>107-08-4</td>
<td>C$_3$H$_7$I</td>
<td>169.992</td>
<td>–101.3</td>
<td>102.5</td>
<td>1</td>
<td>97.20</td>
</tr>
<tr>
<td>2-Iodopropane</td>
<td>75–30–9</td>
<td>C$_3$H$_7$I</td>
<td>169.992</td>
<td>–90</td>
<td>89.5</td>
<td>1</td>
<td>99.75</td>
</tr>
<tr>
<td>1-Iodobutane ($n$-Butyl iodide)</td>
<td>542-69-8</td>
<td>C$_4$H$_9$I</td>
<td>184.018</td>
<td>–103</td>
<td>130.5</td>
<td>1</td>
<td>113.91</td>
</tr>
<tr>
<td>1-Iodopentane</td>
<td>628–17–1</td>
<td>C$<em>5$H$</em>{11}$I</td>
<td>198.045</td>
<td>–85.6</td>
<td>157.0</td>
<td>1</td>
<td>130.63</td>
</tr>
<tr>
<td><strong>Mixed halogenated hydrocarbons:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bromochloromethane</td>
<td>74-97-5</td>
<td>CH$_2$BrCl</td>
<td>129.384</td>
<td>–87.9</td>
<td>68.0</td>
<td>1</td>
<td>66.89</td>
</tr>
<tr>
<td>Bromodichloromethane</td>
<td>75-27-4</td>
<td>CHBrCl$_2$</td>
<td>163.829</td>
<td>–57</td>
<td>90</td>
<td>1</td>
<td>83.12</td>
</tr>
<tr>
<td>Dibromochloromethane</td>
<td>124-48-1</td>
<td>CHBr$_2$Cl</td>
<td>208.280</td>
<td>–20</td>
<td>120</td>
<td>1</td>
<td>84.98</td>
</tr>
<tr>
<td>Chlorodifluoromethane (HCFC-22)</td>
<td>75-45-6</td>
<td>CHCIF$_2$</td>
<td>86.469</td>
<td>–157.42</td>
<td>–40.7</td>
<td>1</td>
<td>71.25</td>
</tr>
<tr>
<td>Dichlorodifluoromethane (CFC-12)</td>
<td>75-71-8</td>
<td>CCl$_2$F$_2$</td>
<td>120.914</td>
<td>–158</td>
<td>–29.8</td>
<td>1</td>
<td>90.97</td>
</tr>
<tr>
<td>Trichlorofluoromethane (CFC-11)</td>
<td>75-69-4</td>
<td>CCl$_3$F</td>
<td>137.368</td>
<td>–110.44</td>
<td>23.7</td>
<td>1</td>
<td>92.32</td>
</tr>
<tr>
<td>1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)</td>
<td>76-13-1</td>
<td>C$_3$F$_3$Cl$_3$</td>
<td>187.375</td>
<td>–36.22</td>
<td>47.7</td>
<td>1</td>
<td>119.84</td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)</td>
<td>76–12–0</td>
<td>C$_4$F$_5$Cl$_4$</td>
<td>203.830</td>
<td>24.8</td>
<td>92.8</td>
<td>1</td>
<td>145.4</td>
</tr>
</tbody>
</table>

* Assuming $\Delta S_{\text{ fus }} = 56$ J/mol K.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$P^{l}$/Pa</td>
<td>$P_{l}$/Pa</td>
<td>$S$/(g/m³)</td>
</tr>
<tr>
<td>Chloroalkanes:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chloromethane</td>
<td>570000</td>
<td>570000</td>
<td>5325</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>580000</td>
<td>580000</td>
<td>13200</td>
</tr>
<tr>
<td>Trichloromethane</td>
<td>26200</td>
<td>26200</td>
<td>8200</td>
</tr>
<tr>
<td>Tetrachloromethane</td>
<td>15250</td>
<td>15250</td>
<td>800</td>
</tr>
<tr>
<td>Chloroethene</td>
<td>16000</td>
<td>16000</td>
<td>5700</td>
</tr>
<tr>
<td>1,1-Dichloroethane</td>
<td>30260</td>
<td>30260</td>
<td>5040</td>
</tr>
<tr>
<td>1,2-Dichloroethane</td>
<td>10540</td>
<td>10540</td>
<td>8600</td>
</tr>
<tr>
<td>1,1,1-Trichloroethane</td>
<td>16500</td>
<td>16500</td>
<td>1290</td>
</tr>
<tr>
<td>1,1,2-Trichloroethane</td>
<td>3220</td>
<td>3220</td>
<td>4590</td>
</tr>
<tr>
<td>1,1,1,2-Tetrachloroethane</td>
<td>1580</td>
<td>1580</td>
<td>1070</td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloroethane</td>
<td>793</td>
<td>793</td>
<td>2830</td>
</tr>
<tr>
<td>Pentachloroethane</td>
<td>590</td>
<td>590</td>
<td>490</td>
</tr>
<tr>
<td>Hexachloroethane</td>
<td>50</td>
<td>1923</td>
<td>50</td>
</tr>
<tr>
<td>1-Chloropropane</td>
<td>46000</td>
<td>46000</td>
<td>2500</td>
</tr>
<tr>
<td>2-Chloropropane</td>
<td>68700</td>
<td>68700</td>
<td>3000</td>
</tr>
<tr>
<td>1,2-Dichloropropane</td>
<td>6620</td>
<td>6620</td>
<td>2740</td>
</tr>
<tr>
<td>1,2,3-Trichloropropane</td>
<td>492</td>
<td>492</td>
<td>1896</td>
</tr>
<tr>
<td>1-Chlorobutane</td>
<td>13700</td>
<td>13700</td>
<td>615</td>
</tr>
<tr>
<td>2-Chlorobutane</td>
<td>20210</td>
<td>20210</td>
<td>1000</td>
</tr>
<tr>
<td>1-Chloropentane</td>
<td>4142</td>
<td>4142</td>
<td>198</td>
</tr>
<tr>
<td>Chloroalkenes:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chloroethene</td>
<td>354600</td>
<td>354600</td>
<td>2763</td>
</tr>
<tr>
<td>1,1-Dichloroethene</td>
<td>80500</td>
<td>80500</td>
<td>3344</td>
</tr>
<tr>
<td>cis-1,2-Dichloroethene</td>
<td>27000</td>
<td>27000</td>
<td>3500</td>
</tr>
<tr>
<td>trans-1,2-Dichloroethene</td>
<td>44400</td>
<td>44400</td>
<td>6260</td>
</tr>
<tr>
<td>Trichloroethylene</td>
<td>9900</td>
<td>9900</td>
<td>1100</td>
</tr>
<tr>
<td>Tetrachloroethylene</td>
<td>2415</td>
<td>2415</td>
<td>150</td>
</tr>
</tbody>
</table>

(Continued)
### TABLE 5.2.2 (Continued)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P^a/Pa P^b/Pa</td>
<td>S/(g/m^3) C^a/(mol/m^3) C^b/(mol/m^3) log K_{OW}</td>
<td>H/(Pa·m^3/mol)</td>
</tr>
<tr>
<td>1,3-Dichloropropene</td>
<td>1.98</td>
<td>1.98</td>
<td>1.98</td>
</tr>
<tr>
<td>Chloroprene</td>
<td>23194</td>
<td>23194</td>
<td>23194</td>
</tr>
<tr>
<td>Hexachloro-1,3-butadiene</td>
<td>20.0</td>
<td>20.0</td>
<td>20.0</td>
</tr>
<tr>
<td>Hexachlorocyclopentadiene</td>
<td>10.9</td>
<td>10.9</td>
<td>10.9</td>
</tr>
<tr>
<td><strong>Bromoalkanes and bromoalkenes:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bromomethane</td>
<td>217700</td>
<td>217700</td>
<td>217700</td>
</tr>
<tr>
<td>Dibromomethane</td>
<td>6034</td>
<td>6034</td>
<td>6034</td>
</tr>
<tr>
<td>Tribromomethane</td>
<td>727</td>
<td>727</td>
<td>727</td>
</tr>
<tr>
<td>Bromoethane</td>
<td>62500</td>
<td>62500</td>
<td>62500</td>
</tr>
<tr>
<td>1,2-Dibromoethane</td>
<td>1500</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>1-Bromopropane</td>
<td>18440</td>
<td>18440</td>
<td>18440</td>
</tr>
<tr>
<td>2-Bromopropane</td>
<td>31940</td>
<td>31940</td>
<td>31940</td>
</tr>
<tr>
<td>1,2-Dibromopropane</td>
<td>1040</td>
<td>1040</td>
<td>1040</td>
</tr>
<tr>
<td>1-Bromobutane</td>
<td>5500</td>
<td>5500</td>
<td>5500</td>
</tr>
<tr>
<td>Vinyl bromide</td>
<td>140476</td>
<td>140476</td>
<td>140476</td>
</tr>
<tr>
<td><strong>Iodoalkanes:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iodomethane</td>
<td>54000</td>
<td>54000</td>
<td>54000</td>
</tr>
<tr>
<td>Iodoethane</td>
<td>18160</td>
<td>18160</td>
<td>18160</td>
</tr>
<tr>
<td>1-Iodopropane</td>
<td>5745</td>
<td>5745</td>
<td>5745</td>
</tr>
<tr>
<td>1-Iodobutane</td>
<td>1848</td>
<td>1848</td>
<td>1848</td>
</tr>
<tr>
<td><strong>Mixed halogenated hydrocarbons:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bromochloromethane</td>
<td>19600</td>
<td>19600</td>
<td>19600</td>
</tr>
<tr>
<td>Bromodichloromethane</td>
<td>6670</td>
<td>6670</td>
<td>6670</td>
</tr>
<tr>
<td>Dibromochloromethane</td>
<td>4000</td>
<td>4000</td>
<td>4000</td>
</tr>
<tr>
<td>Chlorodifluoromethane (HCFC-22)</td>
<td>1044000</td>
<td>1044000</td>
<td>1044000</td>
</tr>
<tr>
<td>Dichlorodifluoromethane (CFC-12)</td>
<td>651000</td>
<td>651000</td>
<td>651000</td>
</tr>
<tr>
<td>Trichlorofluoromethane (CFC-11)</td>
<td>102200</td>
<td>102200</td>
<td>102200</td>
</tr>
<tr>
<td>1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)</td>
<td>48320</td>
<td>48320</td>
<td>48320</td>
</tr>
</tbody>
</table>

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m^3/mol) = 101325 Pa/C^a mol/m^3.
### TABLE 5.2.3
Suggested half-life classes of halogenated hydrocarbons in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycloalkanes and cycloalkenes:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Trichloromethane</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Tetrachloroethane</td>
<td>8</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Chloroethane</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2-Dichloroethene</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloroethane</td>
<td>8</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Pentachloroethane</td>
<td>8</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Hexachloroethane</td>
<td>8</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2-Dichloropropane</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,3-Trichloropropane</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Chloroethene (Vinyl chloride)</td>
<td>3</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>Trichloroethylene</td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Tetrachloroethylene</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Chloroprene</td>
<td>3</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>Bromoalkanes and bromoalkenes:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tribromomethane</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Mixed halogenated hydrocarbons:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bromodichloromethane</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>Chlorotrifluoromethane (CFC-11)</td>
<td>8</td>
<td>8</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (h)</th>
<th>Range (h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>&lt; 10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~ 1 d)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~ 2 d)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5500 (~ 8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17,000 (~ 2 yr)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55,000 (~ 6 yr)</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>
**FIGURE 5.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

**FIGURE 5.2.2** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.
FIGURE 5.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

FIGURE 5.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.
**FIGURE 5.2.5** Octanol-water partition coefficient versus Le Bas molar volume for chloroalkanes.

**FIGURE 5.2.6** Octanol-water partition coefficient versus Le Bas molar volume for halogenated aliphatic hydrocarbons.
FIGURE 5.2.7 Henry's law constant versus Le Bas molar volume for chloroalkanes.

FIGURE 5.2.8 Henry's law constant versus Le Bas molar volume for halogenated aliphatic hydrocarbons.
FIGURE 5.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for chloroalkanes.

FIGURE 5.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for halogenated aliphatic hydrocarbons.
5.3 REFERENCES


Bobbo, S., Fedele, L., Camporese, R., Stryjek, R. (2000c) Isothermal vapor-liquid equilibrium for the three binary systems 1,1,1,2,3,3,3-hexafluoropropane (R236fa) + HC-600a + HFC-245fa. *Fluid Phase Equilib.* 60, 504–505.


Bobbo, S., Camporese, R., Zilio, C. (2000b) Isothermal vapor-liquid equilibria for the binary system 1,1,1-trifluoroethane (R143a) + 1,1,1,3,3,3-hexafluoropropane (R236fa) at 283.11, 298.16, and 313.21 K. *J. Chem. Eng. Data* 45, 276–279.

Bobbo, S., Fedele, L., Camporese, R., Stryjek, R. (2000c) Isothermal vapor-liquid equilibrium for the three binary systems 1,1,1,2,3,3,3-hexafluoropropane with dimethyl ether or propane, and 1,1,1,3,3,3-hexafluoropropane with dimethyl ether. *Fluid Phase Equilibria* 174, 3–12.


Halogenated Aliphatic Hydrocarbons

1239


© 2006 by Taylor & Francis Group, LLC


DIPPR Design Institute for Physical Property Data compilation on the Scientific and Technical International Network (STN).


Halogenated Aliphatic Hydrocarbons


Grosse, A.V., Wackher, R.C., Linn, C.B. (1940) Physical properties of the alkyl fluorides and a comparison of the alkyl fluorides with the other halides and with the alkyls of the elements of Period II. J. Phys. Chem. 44, 275–296.


Kasner, J.H., Taylor P.H., Dellinger, B. (1990) Laser photolysis/laser induced fluorescence study of OH-C2H5Cl rate constants from


USEPA (1986) GEMS Graphical Modeling System. CHEMEST.


Halogenated Aliphatic Hydrocarbons


6.1 List of Chemicals and Data Compilations .................................................. 1259

6.1.1 Chlorobenzenes .................................................................................. 1259
  6.1.1.1 Chlorobenzene .............................................................................. 1259
  6.1.1.2 1,2-Dichlorobenzene ................................................................. 1268
  6.1.1.3 1,3-Dichlorobenzene ................................................................. 1278
  6.1.1.4 1,4-Dichlorobenzene ................................................................. 1287
  6.1.1.5 1,2,3-Trichlorobenzene ............................................................. 1305
  6.1.1.6 1,2,4-Trichlorobenzene ............................................................. 1305
  6.1.1.7 1,3,5-Trichlorobenzene ............................................................. 1314
  6.1.1.8 1,2,3,4-Tetrachlorobenzene ...................................................... 1326
  6.1.1.9 1,2,3,5-Tetrachlorobenzene ...................................................... 1330
  6.1.1.10 1,2,4,5-Tetrachlorobenzene ..................................................... 1335
  6.1.1.11 Pentachlorobenzene ................................................................ 1335
  6.1.1.12 Hexachlorobenzene ................................................................ 1343

6.1.2 Chlorotoluenes .................................................................................... 1352
  6.1.2.1 2-Chlorotoluene ....................................................................... 1352
  6.1.2.2 3-Chlorotoluene ....................................................................... 1355
  6.1.2.3 4-Chlorotoluene ....................................................................... 1357
  6.1.2.4 2,4-Dichlorotoluene .................................................................. 1360
  6.1.2.5 2,6-Dichlorotoluene .................................................................. 1362
  6.1.2.6 3,4-Dichlorotoluene .................................................................. 1364
  6.1.2.7 2,3,6-Trichlorotoluene ............................................................... 1365
  6.1.2.8 2,4,5-Trichlorotoluene ............................................................... 1366
  6.1.2.9 α-Chlorotoluene ........................................................................ 1368
  6.1.2.10 α,α,α-Trichlorotoluene ............................................................ 1371
  6.1.2.11 Pentachlorotoluene .................................................................. 1373
  6.1.2.12 α-Chlorostyrene ..................................................................... 1374
  6.1.2.13 m-Chlorostyrene ..................................................................... 1375
  6.1.2.14 p-Chlorostyrene ..................................................................... 1377
  6.1.2.15 Octachlorostyrene .................................................................. 1379

6.1.3 Fluorobenzenes ................................................................................. 1380
  6.1.3.1 Fluorobenzene .......................................................................... 1380
  6.1.3.2 1,2-Difluorobenzene ................................................................. 1384
  6.1.3.3 1,3-Difluorobenzene ................................................................. 1386
  6.1.3.4 1,4-Difluorobenzene ................................................................. 1388
  6.1.3.5 1,2,4-Trifluorobenzene ............................................................. 1390
  6.1.3.6 1,3,5-Trifluorobenzene ............................................................. 1391
  6.1.3.7 1,2,3,4-Tetrafluorobenzene ...................................................... 1393
6.1.3.8 1,2,3,5-Tetrafluorobenzene .......................................................... 1395
6.1.3.9 1,2,4,5-Tetrafluorobenzene .......................................................... 1397
6.1.3.10 Pentafluorobenzene ...................................................................... 1399
6.1.3.11 Hexafluorobenzene ...................................................................... 1401
6.1.3.12 Pentafluorotoluene ...................................................................... 1404
6.1.3.13 Chloropentafluorobenzene ............................................................ 1406
6.1.3.14 Pentfluorophenol ......................................................................... 1408

6.1.4 Bromobenzenes and bromotoluenes ................................................... 1410
6.1.4.1 Bromobenzene .............................................................................. 1410
6.1.4.2 1,2-Dibromobenzene .................................................................... 1416
6.1.4.3 1,3-Dibromobenzene .................................................................... 1418
6.1.4.4 1,4-Dibromobenzene .................................................................... 1420
6.1.4.5 1,2,3-Tribromobenzene .................................................................. 1423
6.1.4.6 1,2,4-Tribromobenzene .................................................................. 1424
6.1.4.7 1,3,5-Tribromobenzene .................................................................. 1425
6.1.4.8 1,2,4,5-Tetrabromobenzene ............................................................ 1427
6.1.4.9 Hexabromobenzene ........................................................................ 1429
6.1.4.10 2-Bromotoluene .......................................................................... 1431
6.1.4.11 3-Bromotoluene .......................................................................... 1433
6.1.4.12 4-Bromotoluene .......................................................................... 1435

6.1.5 Iodobenzenes .................................................................................... 1437
6.1.5.1 Iodobenzene .................................................................................. 1437
6.1.5.2 1,2-Diiodobenzene ....................................................................... 1441
6.1.5.3 1,3-Diiodobenzene ....................................................................... 1442
6.1.5.4 1,4-Diiodobenzene ....................................................................... 1443
6.1.5.5 1,2,3-Triiodobenzene .................................................................... 1444
6.1.5.6 1,2,4-Triiodobenzene .................................................................... 1445
6.1.5.7 1,3,5-Triiodobenzene .................................................................... 1446

6.1.6 Mixed halogenated benzenes .............................................................. 1447
6.1.6.1 2-Bromochlorobenzene .................................................................. 1447
6.1.6.2 3-Bromochlorobenzene .................................................................. 1448
6.1.6.3 4-Bromochlorobenzene .................................................................. 1450
6.1.6.4 4-Bromoiodobenzene ..................................................................... 1453
6.1.6.5 2-Chloroiodobenzene ..................................................................... 1454
6.1.6.6 3-Chloroiodobenzene ..................................................................... 1455
6.1.6.7 4-Chloroiodobenzene ..................................................................... 1456

6.2 Summary Tables and QSPR Plots ......................................................... 1457
6.3 References .......................................................................................... 1463
6.1 LIST OF CHEMICALS AND DATA COMPILATIONS

6.1.1 CHLOROBENZENES

6.1.1.1 Chlorobenzene

![Chemical Structure of Chlorobenzene]

Common Name: Chlorobenzene
Synonym: monochlorobenzene, benzene chloride, phenyl chloride
Chemical Name: chlorobenzene
CAS Registry No: 108-90-7
Molecular Formula: C₆H₅Cl
Molecular Weight: 112.557
Melting Point (°C): –45.31 (Lide 2003)
Boiling Point (°C): 131.72 (Lide 2003)
Density (g/cm³ at 20°C): 1.1058 (Weast 1972–73; Lide 2003)
Molar Volume (cm³/mol):
  101.8 (20°C, calculated-density)
  116.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
Enthalpy of Fusion, ∆Hfus (kJ/mol):
  9.49 (Dean 1985)
  11.88 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

488 (30°C, shake flask-interferometer, Gross & Saylor 1931)
551 (Landolt-Börnstein 1951)
488 (Seidell 1941)
< 200 (residue-volume method, Booth & Everson 1948)
500 (shake flask-UV, Andrews & Keefer 1950)
490* (30°C, shake flask, Kisorov 1962)
546, 523; 534 (21°C, generator column-GC; mean value, Chey & Calder 1972)
463 (shake flask-UV, Vesala 1974)
100 (Stephen & Stephen 1963)
106.8* (shake flask-GC, measured range 5–45°C, Nelson & Smit 1978)
472 (shake flask-GC, Aquan-Yuen et al. 1979)
472 (shake flask-GC, Mackay et al. 1979, 1980, 1982b)
503 (shake flask-UV, Yalkowsky et al. 1979)
420, 450* (20°C; elution chromatography, UV adsorption, measured range 10–30°C, Schwarz & Miller 1980)
295 (generator column-HPLC/UV, Tewari et al. 1982)
498 (recommended, Horvath 1982)
499 (generator column-HPLC/UV, Wasik et al. 1983)
508 (HPLC-k’ correlation, converted from reported γw, HaKenscheid & Tomlinson 1983a)
295 (generator column-GC, Miller et al. 1984, 1985)
495* (recommended, temp range 10–70°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
\[
S/(g/kg) = 11.3351 - 3.0290 \times 10^{-2}(T/K) - 1.8716 \times 10^{-4}(T/K)^2 + 0.559466 \times 10^{-6}(T/K)^3; \text{ temp range 283–363 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)}
\]

490 \hspace{1cm} (30°C, quoted, Dean 1985)

502 \hspace{1cm} (shake flask-HPLC/UV, Banerjee 1984)

348 \hspace{1cm} (shake flask-radiometric method, Lo et al. 1986)

428 \hspace{1cm} (vapor phase saturation-GC, temp range 15–45°C, Sanemasa et al. 1987)

482* \hspace{1cm} (20°C vapor-liquid equilibrium-activity coefficient, measured range 20–50°C, Cooling et al. 1992)

477 \hspace{1cm} (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

333 \hspace{1cm} (shake flask-GC, Boyd et al. 1998)

496 \hspace{1cm} (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

\[
\ln x = -41.9062 + 6054.03/(T/K) + 1.3692 \times 10^{-4}(T/K)^2; \text{ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)}
\]

470* \hspace{1cm} (shake flask-GC, measured range 5–45°C, Ma et al. 2001)

426, 427, 511 (5, 15, 35°C, estimated-RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

1333* (22.2°C, summary of literature data, temp range –13.0 to 132.2°C, Stull 1947)

\[
\log (P/mmHg) = 7.18473 - 1556.6/(230 + t/°C) \text{ (Antoine eq., Dreisbach & Martin 1949)}
\]

\[
\log (P/mmHg) = 6.94504 - 1413.12/(216.0 + t/°C) \text{; temp range 40–200°C (Antoine eq. for liquid state, Dreisbach 1955)}
\]

7605* \hspace{1cm} (56.28°C, ebulliometry, measured range 56.28–131.70°C, Dreisbach & Shadrer 1949)

9657* \hspace{1cm} (62.04°C, ebulliometry, measured range 62.04–131.7°C, Brown 1952)

1580 \hspace{1cm} (interpolated-Antoine eq., Weast 1972–73)

\[
\log (P/mmHg) = [-0.2185 \times 10098.0/(T/K)] + 8.5000; \text{ temp range –35 to –15°C (Antoine eq., Weast 1972–73)}
\]

\[
\log (P/mmHg) = [-0.2185 \times 9067.3/(T/K)] + 7.71755; \text{ temp range –13 to 249.8°C (Antoine eq., Weast 1972–73)}
\]

1596, 1610 \hspace{1cm} (extrapolated-Antoine eq., Boublik et al. 1973; 1984)

\[
\log (P/kPa) = 6.07963 - 1419.45/(216.33 + t/°C); \text{ temp range 62.04–131.7°C (Antoine eq. from reported exp. data, Boublik et al. 1984)}
\]

\[
\log (P/mmHg) = 6.97808 - 1431.05/(217.65 + t/°C); \text{ temp range 62–131.7°C (Antoine eq., Dean 1985, 1992)}
\]

1596 \hspace{1cm} (extrapolated, Antoine eq., Daubert & Danner 1985)

1596 \hspace{1cm} (extrapolated, Antoine eq., Dean 1985)

\[
\log (P/mmHg) = 6.97808 - 1431.05/(217.65 + t/°C); \text{ temp range 62–131.7°C (Antoine eq., Dean 1985, 1992)}
\]

1600 \hspace{1cm} (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/kPa) = 6.11512 - 1438.86/(-54.72 + T/K); \text{ temp range 333–405 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P/kPa) = 6.62988 - 1897.41/(5.21 + T/K); \text{ temp range 405–597 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

1410* \hspace{1cm} (gas saturation-GC, measured range –14.2 to 40°C, Liu & Dickhut 1994)

828; 1560 \hspace{1cm} (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)

\[
\log (P/mmHg) = 19.4343 - 2.5801 \times 10^{-3}/(T/K) - 3.9391 \log (T/K) - 4.4005 \times 10^{-11}/(T/K)^2 + 4.9583 \times 10^{-7}/(T/K)^3; \text{ temp range 228–632 K (Yaws 1994)}
\]

\[
\log P/kPa = 6.11512 - 1438.86/(T/K - 54.72); \text{ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

451 \hspace{1cm} (calculated as I/K_{AW}, C_W/C_A, reported as exp. lit., Hine & Mookerjee 1975)

441 \hspace{1cm} (calculated-bond contribution, Hine & Mookerjee 1975)

382 \hspace{1cm} (batch stripping-GC, Mackay et al. 1979)

379 \hspace{1cm} (calculated P/C, Mackay et al. 1979)

330* \hspace{1cm} (equilibrium cell-concentration ratio, measured range 1.0–23.0°C, Leighton & Calo 1981)

\[
\ln (k_H/atm) = 16.83 - 3466/(T/K); \text{ temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)}
\]

314 \hspace{1cm} (batch air stripping-GC, Mackay & Shiu 1981)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

- 398 (gas stripping-GC, Warner et al. 1987)
- 319 (20°C, EPICS-GC, Yurteri et al. 1987)
- 273 (20°C, calculated-P/C, Yurteri et al. 1987)
- \( \ln \left[ \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right] = 3.469 - \frac{2689}{(T/\text{K})} \); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 460 (computer value, Yaws et al. 1991)
- 324* (extrapolated from equilibrium headspace-GC data, measured range 45–80°C, Ettre et al. 1993)
- \( \log (1/K_{AW}) = -2.9050240 + \frac{1129.8083}{(T/\text{K})} \); temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
- 288 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
- 315 (gas stripping-GC, Shiu & Mackay 1997)
- 293 (headspace equilibrium-GC, de Wolf & Lieder 1998)
- 277.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
- 537 (modified EPICS method-GC, Ryu & Park 1999)
- 297 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
- \( \log K_{AW} = 4.225 - \frac{1507}{(T/\text{K})} \) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
- 384* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
- \( \ln K_{AW} = 10.04 - \frac{3359.7}{(T/\text{K})} \); temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, \( \log K_{OW} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
- 2.84 (Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1985)
- 2.81 (calculated-fragment constant, Rekker 1977)
- 2.18 (\(^{14}\text{C}-\text{LSC}, \text{Lu} \& \text{Metcalf 1975})
- 2.84, 2.46, 2.18 (Hansch & Leo 1979)
- 2.79 (HPLC-RT correlation, Veith et al. 1979b)
- 2.84 (HPLC-k’ correlation, Könemann et al. 1979)
- 2.80 (HPLC-k’ correlation, Hanai et al. 1981)
- 2.81 (HPLC-k’ correlation, D’Amboise & Hanai 1982)
- 2.83 (shake flask-HPLC, Hammers et al. 1982)
- 2.18 (HPLC-k’ correlation, Miyake & Terada 1982)
- 2.80 (HPLC-k’ correlation, Hafkenscheid & Tomlinson 1983a)
- 2.98 (generator column-HPLC/UV, Wasik et al. 1983)
- 2.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
- 2.81–2.84 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
- 2.49 (HPLC-k’ correlation, Haky & Young 1984)
- 3.00 (HPLC-k’ correlation, De Kock & Lord 1987)
- 2.898 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 2.784 ± 0.061, 2.898 ± 0.004 (shake flask methods, interlaboratory studies, Brooks et al. 1990)
- 2.65, 2.73; 2.84 (25°C, 60°C, shake flask-UV/VIS; quoted lit. at 25°C, Kramer & Henze 1990)
- 2.86, 3.02 (centrifugal partition chromatography, Gluck & Martin 1990)
- 2.84 (recommended, Sangster 1993)
- 2.89 (recommended, Hansch et al. 1995)
- 2.98 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
- 2.96 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)
- 3.05* (estimated-RP-HPLC-k’ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
- 3.45* (20°C, HPLC-k’ correlation, measured range 10–50°C, Su et al. 2002)
- \( \log K_{OA} = 43910/(2.303 \cdot RT) - 4.107 \); temp range 10–50°C (HPLC-k’ correlation, Su et al. 2002)

Bioconcentration Factor, \( \log BCF \):
- 2.65 (fathead minnow, Veith et al. 1979b, 1980)
- 1.30 (Kenaga 1980a)
Sorption Partition Coefficient, log $K_{OC}$:

- 2.52 (sediment, Mabey et al. 1982)
- 2.18 (Kenaga 1980a)
- 2.59 (field data, Roberts et al. 1980; Schwarzenbach & Westall 1981; quoted, Voice & Weber 1985)
- 1.84 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 1.73–2.99 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.44, 2.50 (calculated from $K_{OFO}$, Schwarzenbach & Westall 1981)
- 2.73 (soil, calculated-$K_{OFO}$, Calamari et al. 1983)
- 2.10 (calculated-MCI $\chi$, Koch 1983)
- 2.92 (calculated-$K_{OFO}$, Yoshida et al. 1983b)
- 2.60 (Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber, Jr. 1985)
- 2.44 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 1.92–2.59 (soil, Howard 1989)
- 2.50; 2.17 (Captina silt loam, OC 1.49%, pH 4.17; McLaurin sandy loam, OC 0.66%, pH 4.42, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 2.34 (calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.19, 2.20 (RP-HPLC-k’ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.97, 2.14, 1.77 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log $K_{OM}$:

- 1.68 (Woodburn soil, organic matter 1.9%, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
- 2.10, 2.32 (quoted, calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- Volatilization: estimated $t_{1/2}$ ~ 1–12 h from a flowing stream (Cadena, 1984; selected, Howard 1989);
  $k = 0.033$ d$^{-1}$ with $t_{1/2} = 21$ d in spring at 8–16°C, $k = 0.152$ d$^{-1}$ with $t_{1/2} = 4.6$ d in summer at 20–22°C, $k = 0.053$ d$^{-1}$ with $t_{1/2} = 13$ d in winter at 3–7°C for periods when volatilization appears to dominate, and $k = 0.08$ d$^{-1}$ with $t_{1/2} = 8.9$ d with HgCl$_2$ in September 9–15, 1980 in marine mesocosm experiments; estimated half-lives from soil: $t_{1/2} = 0.3$ d of 1-cm depth and $t_{1/2} = 12.6$ d for 10 cm depth (Wakeham et al. 1983).
- Photolysis: not environmentally significant or relevant (Mabey et al. 1982); photolysis $k = 1.1 \times 10^{-5}$ d$^{-1}$ with an estimated $t_{1/2}$ ~170 yr by sunlight in surface water at 40°N in the summer (Dulin et al. 1986)
  $t_{1/2} = 21$ d under sunlight in water (Mansour & Feicht 1994).
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
  photooxidation $t_{1/2} = 1553–62106$ h in water, based on a measured rate for hydroxy radicals in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)
  $k_{OH} = 9.0 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 13 d, loss of 7.4% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
  $k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k << 1$ M$^{-1}$ h$^{-1}$ for RO$_2$ radical (Mabey et al. 1982)
  $k = (0.75 \pm 0.2)3$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)
k = 2.88 × 10⁻³ h⁻¹ in air (Yoshida et al. 1983b; selected, Mackay et al. 1985)
kOH = (8.8 ± 1) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with estimated atmospheric lifetime τ = 13 d and kO₃ < 5 × 10⁻²¹ cm³ molecule⁻¹ s⁻¹ with lifetime τ > 8.8 yr at room temp. (relative rate method, Atkinson et al. 1985)
kOH (obs.) = 9.4 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹; and kOH(calc) = 1.6 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)

kOH = (5.5 ± 4.4) × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 23.5°C with an atmospheric lifetime τ = 21 d (relative rate method, Edney et al. 1986)
kOH = 9.4 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ with t½ = 17 d for reaction with OH radical, concn of 5.0 × 10⁵ molecule/cm³ at room temp. (Atkinson 1987)
kOH(calc) = 1.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, kOH(obs) = 0.71 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)

kOH(calc) = 7.7 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)
kOH(calc) = 0.70 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);
base rate constant k < 0.9 M⁻¹ h⁻¹ with t½ > 900 yr, based on assumed base mediated 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988).
t½ > 879 yr based on rate constant k < 0.9 M⁻¹ h⁻¹ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988)

Biodegradation: significant degradation on anaerobic environment with k = 0.5 d⁻¹ (Tabak et al. 1981; Mills et al. 1982)
k = 1.88 × 10⁻⁴ h⁻¹ in air, and k = 3.83 × 10⁻⁴ h⁻¹ in sediments (Lee & Ryan 1979; selected, Mackay et al. 1985)
k = 0.24 L d⁻¹ in air, no degradation in water and on the ground (Neely 1982);
k = 0.07–0.3 d⁻¹ in river water; k = 0.04–0.2 d⁻¹ in estuary water; and k = 0.01 d⁻¹ in marine water (Bartholomew & Pfaender 1983; selected, Batterby 1990)
k = 0.033 d⁻¹, t½ = 21 d in spring at 8–16°C, k = 0.152 d⁻¹, t½ = 4.6 d in summer at 20–22°C, k = 0.053 d⁻¹, t½ = 13 d in winter at 3–7°C, and k = 0.08 d⁻¹, t½ = 8.9 d with HgCl₂ in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983)
t½ = 4.6–21 d in marine mesocosm (Wakeham et al. 1983);
t½ = 7.9 d in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991);
k = 0.07 yr⁻¹ with t½ = 37 d (Olsen & Davis 1990)
t½(aq. aerobic) = 1632–3600 h, based on unacclimated aerobic river dieaway tests; t½(aq. anaerobic) = 6528–14400 h, based on estimated aequous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation: 3 × 10⁻⁹ mL cell⁻¹ h⁻¹ (estimated, Mabey et al. 1982).
Bioconcentration, Uptake (kₜ), and Elimination (kₑ) Rate Constants:

Half-Lives in the Environment:
Air: photodecomposition t½ = 8.7 h under simulated atmospheric conditions, with NO (Dilling et al. 1976); residence time of 13 d, loss of 7.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
estimated atmospheric lifetime τ = 13 d due to reaction with OH radical and τ > 8.8 yr due to reaction with O₃ (Atkinson et al. 1985);
t₀ = 72.9–729 h, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water: t½ = 0.3 d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)
t½ = 75 d for an estuarine river with near natural conditions at 22°C (Lee & Ryan 1976);
rate constants: k = 0.033 d⁻¹, t½ = 21 d in spring at 8–16°C, k = 0.152 d⁻¹, t½ = 4.6 d in summer at 20–22°C,
k = 0.053 d⁻¹, t½ = 13 d in winter at 3–7°C for periods when volatilization appears to dominate, and k = 0.08 d⁻¹, t½ = 8.9 d with HgCl₂ in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983)
$t_{1/2} = 1632–3600 \text{ h}$, based on unacclimated aerobic river dieaway tests (Howard et al. 1991).

Photolysis $t_{1/2} = 21 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).

Groundwater: $t_{1/2} = 3264–7200 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 75 \text{ d}$ (Lee & Ryan 1976, 1979; quoted, Anderson et al. 1991).

Soil: disappearance $t_{1/2} = 2.1 \text{ d}$ from testing soils (Anderson et al. 1991);

$\text{Soil: } t_{1/2} = 1632–3600 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 6.1.1.1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities of chlorobenzene at various temperatures</td>
</tr>
</tbody>
</table>

1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask</td>
<td>vapor equil.-UV spec.</td>
<td>elution chromatography</td>
<td>recommended values</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
</tr>
<tr>
<td>30</td>
<td>490</td>
<td>5</td>
<td>40</td>
</tr>
<tr>
<td>40</td>
<td>705</td>
<td>25</td>
<td>106.8</td>
</tr>
<tr>
<td>50</td>
<td>960</td>
<td>35</td>
<td>400.5</td>
</tr>
<tr>
<td>60</td>
<td>1100</td>
<td>45</td>
<td>471.3</td>
</tr>
<tr>
<td>70</td>
<td>1605</td>
<td>10</td>
<td>460</td>
</tr>
<tr>
<td>80</td>
<td>1805</td>
<td>20</td>
<td>450</td>
</tr>
<tr>
<td>90</td>
<td>2500</td>
<td>30</td>
<td>500</td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>Cooling et al. 1992</th>
<th>Ma et al. 2001</th>
<th>Finizio &amp; Di Guardo 2001</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC/MS</td>
<td>shake flask-GC</td>
<td>RP-HPLC-k correlation</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>20</td>
<td>482</td>
<td>5</td>
</tr>
<tr>
<td>30</td>
<td>608</td>
<td>15</td>
</tr>
<tr>
<td>40</td>
<td>840</td>
<td>25</td>
</tr>
<tr>
<td>50</td>
<td>1263</td>
<td>35</td>
</tr>
</tbody>
</table>
FIGURE 6.1.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.2
Reported vapor pressures of chlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/^\circ C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/^\circ C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/^\circ C$</td>
<td>$P$/Pa</td>
<td>$t/^\circ C$</td>
<td>$P$/Pa</td>
</tr>
<tr>
<td>–13.0</td>
<td>133.3</td>
<td>–13.0</td>
<td>56.28</td>
</tr>
<tr>
<td>10.6</td>
<td>666.6</td>
<td>10.6</td>
<td>63.05</td>
</tr>
<tr>
<td>22.2</td>
<td>1333</td>
<td>22.2</td>
<td>75.22</td>
</tr>
<tr>
<td>35.3</td>
<td>2666</td>
<td>35.3</td>
<td>101.85</td>
</tr>
<tr>
<td>49.7</td>
<td>5333</td>
<td>49.7</td>
<td>117.30</td>
</tr>
<tr>
<td>58.3</td>
<td>7999</td>
<td>58.3</td>
<td>131.70</td>
</tr>
<tr>
<td>70.0</td>
<td>13332</td>
<td>70.0</td>
<td>131.70</td>
</tr>
<tr>
<td>89.4</td>
<td>26664</td>
<td>89.4</td>
<td>131.70</td>
</tr>
<tr>
<td>110</td>
<td>53329</td>
<td>110</td>
<td>mp/$^\circ C$</td>
</tr>
<tr>
<td>132.2</td>
<td>101325</td>
<td>132.2</td>
<td>bp/$^\circ C$</td>
</tr>
<tr>
<td>$mp/^\circ C$</td>
<td>–45.2</td>
<td>A</td>
<td>7.18473</td>
</tr>
<tr>
<td>B</td>
<td>1556.6</td>
<td>B</td>
<td>1444.75</td>
</tr>
<tr>
<td>C</td>
<td>230</td>
<td>C</td>
<td>219.13</td>
</tr>
</tbody>
</table>
FIGURE 6.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.3
Reported Henry’s law constants of chlorobenzene at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \quad (1) \\
\ln (1/K_{AW}) &= A - B/(T/K) \quad (2) \\
\ln k_H &= A - B/(T/K) \quad (3) \\
\ln H &= A - B/(T/K) \quad (4) \\
K_{AW} &= A - B/(T/K) + C/(T/K)^2 \quad (5)
\end{align*}
\]

1.

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>124</td>
<td>10</td>
<td>247</td>
<td>45</td>
<td>621</td>
<td>2</td>
<td>112</td>
</tr>
<tr>
<td>3</td>
<td>125</td>
<td>15</td>
<td>285</td>
<td>60</td>
<td>863</td>
<td>6</td>
<td>155.5</td>
</tr>
<tr>
<td>12.4</td>
<td>190</td>
<td>20</td>
<td>346</td>
<td>70</td>
<td>1114</td>
<td>10</td>
<td>183.6</td>
</tr>
<tr>
<td>12.5</td>
<td>206</td>
<td>25</td>
<td>365</td>
<td>80</td>
<td>1579</td>
<td>18</td>
<td>283.2</td>
</tr>
<tr>
<td>17.9</td>
<td>243</td>
<td>30</td>
<td>479</td>
<td></td>
<td></td>
<td>25</td>
<td>384</td>
</tr>
<tr>
<td>19.1</td>
<td>280</td>
<td>30</td>
<td>479</td>
<td></td>
<td></td>
<td>30</td>
<td>472.8</td>
</tr>
<tr>
<td>22.7</td>
<td>271</td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>eq. 2a</td>
<td>1/K_{AW}</td>
<td>40</td>
<td>755.8</td>
</tr>
<tr>
<td>23</td>
<td>321</td>
<td>A</td>
<td>3.469</td>
<td>A</td>
<td>2.905024</td>
<td>50</td>
<td>1046</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>2689</td>
<td></td>
<td>B</td>
<td>1129.8083</td>
<td>60</td>
<td>1420</td>
</tr>
<tr>
<td>eq. 3</td>
<td>k_H/atm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>70</td>
<td>1804</td>
</tr>
<tr>
<td>A</td>
<td>18.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3751</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
FIGURE 6.1.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.4
Reported octanol-water and octanol-air partition coefficients of chlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>log K\text{OW}</th>
<th>log K\text{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finizio &amp; Di Guardo 2001</td>
<td>Su et al. 2002</td>
</tr>
<tr>
<td>GC-RT correlation</td>
<td>GC-RT correlation</td>
</tr>
<tr>
<td>t/°C</td>
<td>log K\text{OW}</td>
</tr>
<tr>
<td>5</td>
<td>3.19</td>
</tr>
<tr>
<td>15</td>
<td>3.15</td>
</tr>
<tr>
<td>25</td>
<td>3.05</td>
</tr>
<tr>
<td>35</td>
<td>3.04</td>
</tr>
<tr>
<td>50</td>
<td>2.65</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 43.91 \]

\[ \log K_{\text{OA}} = A + B/T \]

A = \quad -4.107

B = \quad 43910

FIGURE 6.1.1.4 Logarithm of K\text{OW} and K\text{OA} versus reciprocal temperature for chlorobenzene.
6.1.1.2 1,2-Dichlorobenzene

Common Name: 1,2-Dichlorobenzene
Synonym: o-dichlorobenzene, dowtherm E
Chemical Name: 1,2-dichlorobenzene
CAS Registry No: 95-50-1
Molecular Formula: C₆H₄Cl₂
Molecular Weight: 147.002
Melting Point (°C):
  -17.0 (Pirsch 1956; Dreisbach 1955; Weast 1972–73; 1982–83; Lide 2003)
Boiling Point (°C):
  180 (Lide 2003)
Density (g/cm³ at 20°C):
  1.3048 (Weast 1972–73; Horvath 1982)
  1.3059 (Lide 2003)
Molar Volume (cm³/mol):
  112.6 (20°C, calculated-density)
  137.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  12.93 (Weast 1972–73)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  50.46 (Pirsch 1956)
  50.63 (Yalkowsky & Valvani 1980)
Entropy of Fusion, ΔSfus (J/mol K):
  92.7 (Landolt-Börnstein 1951)
Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  145* (volumetric, measured range 20–60°C, Klemenc & Low 1930; Seidell 1941)
  < 260 (residue-volume method, Booth & Everson 1948)
  92.7 (Landolt-Börnstein 1951)
  79.0 (shake flask-radiolabeled ¹⁴C-LSC, Metcalf et al. 1975)
  148* (20°C, shake flask-GC/ECD, measured 0–34°C, Chiou & Freed 1977)
  92.8 (shake flask-UV, Yalkowsky et al. 1979)
  154 (shake flask-LSC/¹⁴C, Veith et al. 1980)
  127, 124* (20°C; elution chromatography, UV, Schwarz & Miller 1980)
  155.8 (shake flask-LSC, Banerjee et al. 1980; Banerjee 1985)
  149.1 (shake flask-GC, Königmann 1981)
  92.6 (recommended, Horvath 1982)
  125 (quoted average, Yalkowsky et al. 1983)
  92.3 (generator column-GC, Miller et al. 1984, 1985)
  137 (shake flask-HPLC, Banerjee 1984)
  147* (recommended, temp range 0–60°C, IUPAC Solubility Data Series, Hovath & Getzen 1985)

\[
S/(g/kg) = 19.2314 - 1.81140 \times 10^{-1} \cdot (T/K) + 5.6509 \times 10^{-4} \cdot (T/K)^2 - 5.77683 \times 10^{-7} \cdot (T/K)^3, \text{ temp range 273–333 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)}
\]

169 (shake flask-radiometry, Lo et al. 1986)
156 (quoted lit. average, Riddick et al. 1986; Howard 1989)
31* (19.5°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1992)
145 (dialysis tubing equilibration-GC. Etzweiler et al. 1995)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

159.2 (shake flask-GC/ECD, Tam et al. 1996)
144 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
109 (shake flask-GC, Boyd et al., 1998)
92, 93, 137; 97 (quoted lit. values; solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
\[ \ln x = -31.5289 + 3834/(T/K) + 8.7172 \times 10^{-5} \cdot (T/K)^2; \text{ temp range } 5–50°C \] (regression eq. from literature data, Shiu & Ma 2000)
149* ± 8.2 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
140, 124, 158 (5, 15, 25°C, estimated-RP-HPLC-k’ correlation, Finizio & Di Guardo 2001)
93.7* (generator column-GC/ECD, measured range 15–55°C, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

137* (20°C, summary of literature data, Stull 1947)
\[ \log (P/mmHg) = 7.32585 – 1824.6/(230 + t/°C) \] (Antoine eq., Dreisbach & Martin 1949)
5010* (56.28°C, ebulliometry, measured range 87.02–180.48°C, Dreisbach & Shrader 1949)
171 (calculated by formula., Dreisbach 1955)
\[ \log (P/mmHg) = 6.92400 – 1599.034/(206.964 + t/°C) \] (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
25234* (130.82°C, ebulliometry, measured range 130.82–181.62°C, McDonald et al. 1959)
196 (extrapolated, Antoine eq., Weast 1972–73)
\[ \log (P/mmHg) = [-0.2185 \times 10^493.0/(T/K)] + 8.185275; \text{ temp range 20–179°C} \] (Antoine eq., Weast 1972–73)
224.87*; 132, 188 (27.8°C reported; 20°C, 25°C, extrapolated-Antoine eq. from gas saturation-GC measurement, temp range 27.8–70°C, Grayson & Fosbraey 1982)
\[ \log (P/Pa) = 25.4 – 6013/(T/K), \text{ temp range 27.8–70°C} \] (gas saturation-GC, Grayson & Fosbraey 1982)
\[ \log (P/kPa) = 6.26918 – 1705.55/(T/K) \] (liquid, Antoine eq., Stephenson & Malanowski 1987)
164* (gas saturation, measured range –15 to 40°C, Liu & Dickhut 1994)
137.3*; 188 (pressure gauge measured at 20.35°C, 25°C, interpolated from reported Antoine eq., Polednicek et al. 1996)
\[ \ln (P/Pa) = 21.5929 – 4053.86/[T/(K) – 50.2328]; \text{ temp range 256–422 K} \] (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
252; 185 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
\[ \log (P/mmHg) = 31.3614 – 3.5226 \times 10^3/(T/K) – 7.8886-log (T/K) – 2.2250 \times 10^{-10} \cdot (T/K)^2, \text{ temp range 256–705 K} \] (Yaws 1994)
133.8* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)
\[ \ln [(P/Pa)/6.80] = [1 – (T/K)/256.10-\exp{3.359374 – 8.564122 \times 10^{-4} \cdot (T/K) + 6.0235167 \times 10^{-7} \cdot (T/K)^2}]; \text{ temp range 256–445 K} \] (Cox eq., recommended, Roháč et al. 1999)
\[ \log (P/kPa) = 19.40 – 6013/(T/K); \text{ temp range 5–50°C} \] (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.): 248 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
375 (calculated-bond contribution, Hine & Mookerjee 1975)
193 (batch air stripping-GC, Mackay & Shiu 1981)
122 (20°C, gas stripping-GC, Oliver 1985)
Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.55 (Hansch et al. 1968)
- 3.38 (Leo et al. 1971; Hansch & Leo 1979, 1985)
- 3.57 (calculated-fragment constants, Rekker 1977)
- 3.55, 3.39 (shake flask-GC, HPLC-$k'\,,$ Könenmann et al. 1979)
- 3.40; 3.75 (concentration ratio; HPLC-RT correlation, Veith et al. 1980)
- 3.40 (shake flask-LSC, Banerjee et al. 1980)
- 3.71, 3.18–4.36 (shake flask method: mean, range of mean values, OECD 1981)
- 3.34 (shake flask-HPLC, Hammers et al. 1982)
- 3.40 (shake flask-GC, Watarai et al. 1982)
- 3.19, 3.31, 3.53, 3.60, 3.84, 4.15, 4.36; 3.61 (shake flask; results of OECD/EEC laboratory comparison tests; mean value, Harnisch et al. 1983)
- 3.34, 3.20; 3.61 (HPLC methods; OECD/EEC shake-flask method; Harnisch et al. 1983)
- 3.38 (generator column-HPLC/UV, Wasik et al. 1983)
- 3.38 (generator column-GC, Miller et al. 1984, 1985)
- 3.56 (HPLC-RV correlation, Garst 1984)
- 3.433 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 3.49 (shake flask-GC, Pereira et al. 1988)
- 3.38 (recommended, Sangster 1993)
- 3.43 (recommended, Hansch et al. 1995)
- 3.29 ± 0.05 (shake flask-GC/ECD, Bahadur et al. 1997)
- 3.29* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)

$$\log K_{OW} = 0.1831 + \frac{17800}{2.303\cdot R(T/K)}; \text{ temp range 5–45°C (van’t Hoff eq., Bahadur et al. 1997)}$$

3.447 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
- 3.70 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrädter 1999)

Octanol/Air Partition Coefficient, log $K_{OA}$ and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.36*, 4.41 (generator column-GC, measured range −10 to 20°C; calculated, Harner & Mackay 1995)

$$\log K_{OA} = -4.30 + 2574.0/(T/K); \Delta H_{OA} = 49.3 \text{ kJ/mol (generator column-GC, Harner & Mackay 1995)}$$
- 4.68 (solid-phase microextraction SPME-GC, Treves et al. 2001)

$$\log K_{OA} = -7.90 + 3304/(T/K), \Delta H_{OA} = 63.3 \text{ kJ/mol (SPME-GC, Treves et al. 2001)}$$

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 1.95 (bluegill sunfish, Veith et al. 1979b; 1980)
- 2.19–2.48 (fish, calculated, Veith et al. 1980)
- 1.95 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 2.86 (microorganisms-water, Mabey et al. 1982)
- 2.40–2.48 mean 2.43; 2.60–2.85 mean 2.74 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 3.51–3.80 (rainbow trout, lipid-basis, Oliver & Niimi 1983)
- 2.43–2.75 (fish, Oliver 1984)
- 1.95 (correlated-flow through method, bluegill sunfish, Davis & Dobbs 1984)
1.60 (fish-normalized, Tadokoro & Tomita 1987)
1.89 (fish, calculated-MCI χ, Sabljic 1987b)
3.94, 4.46, 3.79, 3.82 (field data: Atlantic croaker, blue crabs, spotted sea trout, blue catfish, lipid-based, Pereira et al. 1988)
2.4 ± 0.1 (guppies, steady-state conditions, rate const. ratio k₁/k₂, 96-h exposure, Sijm et al. 1993)
3.5 ± 0.1 (guppies, lipid normalized BCF, Sijm et al. 1993)
2.70 (fathead minnow, steady-state conditions, rate const. ratio k₁/k₂, 96-h exposure, Sijm et al. 1993)
3.90 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)
1.95; 2.43, 2.75 (Lepomis macrochirus; Oncorhynchus mykiss, quoted lit., flow through conditions, Devillers et al. 1996)
2.40; 2.70 (Poecilia reticulata; Pimephales promelas, quoted lit., static and semi-static conditions, Devillers et al. 1996)
2.43, 3.51; 2.333, 2.549 (quoted: whole fish, lipid content; calculated-MCI χ, calculated-Kow, Lu et al. 1999)
3.86; 3.84 (Oncorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log KOC:
2.26 (Willamette silt loam soil, 1.6% organic matter, equilibrium sorption isotherm measurement, Chiou et al. 1979)
3.0, 2.96, 2.62 (calculated-Kow solubility C₁, C₃, Karickhoff 1981)
4.60; 4.60; 3.00 (field data of sediment trap material, Niagara River organic matter, calculated from Kow, Oliver & Charlton 1984)
2.34, 2.59 (Lula aquifer 0.032% OC, Apalachic soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
2.45 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.27, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.43 (untreated Marlette soil B horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
3.64, 3.52 (organic cations treated Marlette soil B horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.45–3.51 (aquifer materials, Stauffer et al. 1989)
3.10, 2.90; 2.99 (Captina silt loam, OC 1.49% and pH 4.97, McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
2.36–2.61 (16 U.S. soils, 1.03–6.09% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.37–2.51 (16 Chinese soils, 0.16–5.61% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.48–2.76 (14 U.S. bed sediments, 0.4–2.20% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.62–2.78 (21 Chinese bed sediments, 0.11–4.73% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.36–2.63 (suspended solids from four U.S. rivers, 1.78–2.87% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.48 (suspended solids from Yellow River, China, 0.30% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
2.39, 2.40 (RP-HPLC-k’ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
3.69 ± 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
2.50, 2.50, 2.47 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
2.70, 2.69, 2.71 (sediments, organic carbon OC ≤ 0.1%, OC ≤ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Coefficient, log KOM:
2.25 (Willamette silt loam soil, 1.6% organic matter, equilibrium isotherm, Chiou et al. 1979; quoted, Howard 1989)
2.27 (Woodburn silt loam soil, 1.9% organic matter, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
2.50 (soil, Chiou et al. 1983)
2.26, 2.54 (quoted, calculated-MCI χ, Sabljic 1984)
2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

2.97 (untreated Marlette soil B horizon, OM 0.60%, equilibrium isotherm, Lee et al. 1989)

3.97, 3.50, 2.87 (organic cations treated Marlette soil B horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives, t½:

Volatilization/Evaporation: experimental evaporation rate into air, $1.18 \times 10^{-6}$ g cm$^{-2}$ s$^{-1}$ (Chiou et al. 1980); estimated $t_{1/2} = 4.4$ h for a model river of 1-m depth with a flow rate of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant (Mabey et al. 1982); rate constant $k = 1.22 \times 10^{-4}$ h$^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical, and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH} \sim 3.0 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $<< 1$ M$^{-1}$ h$^{-1}$ for RO$_2$ radical (Mabey et al. 1982)

$k_{OH} = (4.2 \pm 0.2) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{O3} = 2.0 \times 10^{-23}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298–323 K (Atkinson & Carter 1984)

$k_{OH}(obs.) = 4.2 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; and $k_{OH}(calc) = 4.9 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(calc) = 4.1 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs) = 4.2 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 4.07 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 22–27°C (Dilling et al. 1988)

$k = (3.7–4.0) \times 10^{9}$ M$^{-1}$ s$^{-1}$ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{OH}(calc) = 4.0 \times 10^9$ M$^{-1}$ s$^{-1}$ in aqueous solutions (Haag & Yao 1992)

$k_{OH}(calc) = 0.48 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982).

base rate constant k < 0.9 M$^{-1}$ h$^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

Biodegradation: $t_{1/2}(aq.~aerobic) = 672–4320$ h, based on unacclimated soil grab sample data, and aerobic screening test data (Howard et al. 1991);

$\sim 2880–17280$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991);

significant degradation in an aerobic environment with k = 0.05 d$^{-1}$ (Tabak et al. 1981; Mills et al. 1982);

in a continuous flow of activated sludge system; virtually 100% (78% biodegradation and 22% stripping) was observed (Kincannon et al. 1983; selected, Howard 1989).

Biotransformation: $1 \times 10^{–10}$ ml cell$^{-1}$ h$^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake ($k_i$), and Elimination ($k_e$) Rate Constants:

$k_i = 870$ L kg$^{-1}$ d$^{-1}$; $k_e = 3.90$ d$^{-1}$ (guppy, 96-h exposure., Sijm et al. 1993)

$k_i = 635$ L kg$^{-1}$ d$^{-1}$; $k_e = 1.40$ d$^{-1}$ (fathead minnow, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 152.8–1528$ h, based on the photooxidation half-life in air. (Howard et al. 1991)

Surface water: $t_{1/2} = 1.2–37$ d estimated from field data at various locations in the Netherlands, $t_{1/2} = 0.3–3$ d for river, $t_{1/2} = 3–30$ d for lakes (Zoeteman et al. 1980)

$\sim 672–4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater: $t_{1/2} = 30–300$ d, estimated from persistence in water (Zoeteman et al. 1980);
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

- \( t_{1/2} \approx 1 \text{ yr} \) estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)
- \( t_{1/2} = 1344–8640 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

**Sediment:**
- \( t_{1/2} = 672–4320 \text{ h} \), based on unacclimated aerobic screening test data (Howard et al. 1991)
- Disappearance \( t_{1/2} = 4.0 \text{ d} \) in testing soils (Anderson et al. 1991).

**Biota:**
- \( t_{1/2} < 1 \text{ d} \) in fish (Veith et al. 1980);
- \( t_{1/2} < 1 \text{ d} \) bluegill sunfish. (Barrows et al. 1980);
- \( t_{1/2} < 5 \text{ d} \) in worms at 8°C (Oliver 1987a);
- Biological half-lives: \( t_{1/2} < 1 \text{ d} \) in trout muscle, \( t_{1/2} < 1 \text{ d} \) in sunfish and \( t_{1/2} < 1 \text{ d} \) in guppy for dichlorobenzenes (Niimi 1987).

### TABLE 6.1.1.2.1

**Reported aqueous solubilities of 1,2-dichlorobenzene at various temperatures**

1. **Klemenc & Löw 1930**
   - Volumetric method
   - \( t/°C \) | \( CS / g \cdot m^{-3} \)
   - 20 | 134
   - 25 | 145
   - 30 | 161
   - 35 | 183
   - 40 | 194
   - 45 | 203
   - 55 | 223
   - 60 | 232

2. **Chiou & Freed 1977**
   - Shake flask-GC
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 0 | 50
   - 19.5 | 31
   - 40 | 17
   - 50 | 24
   - 60.5 | 54
   - 70.7 | 55
   - 80.0 | 91
   - 90.5 | 83

3. **Schwarz & Miller 1980**
   - Elution chromatography
   - \( t/°C \) | \( CS / g \cdot m^{-3} \)
   - 0 | 133
   - 19.5 | 127
   - 25 | 149
   - 35 | 162

4. **Horvath & Getzen 1985**
   - Recommended values
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 0 | 142
   - 5 | 135
   - 10 | 133
   - 15 | 134
   - 20 | 139
   - 25 | 147
   - 30 | 157
   - 35 | 169
   - 40 | 182
   - 45 | 197
   - 50 | 212
   - 55 | 228
   - 60 | 243

5. **Stephenson 1992**
   - Shake flask-GC
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 0 | 50
   - 19.5 | 31
   - 40 | 17
   - 50 | 24
   - 60.5 | 54
   - 70.7 | 55
   - 80.0 | 91
   - 90.5 | 83

6. **Ma et al. 2001**
   - Shake flask-GC/FID
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 0 | 50
   - 19.5 | 31
   - 40 | 17
   - 50 | 24
   - 60.5 | 54
   - 70.7 | 55
   - 80.0 | 91
   - 90.5 | 83

7. **Finizio & Di Guardo 2001**
   - RP-HPLC-\( k' \) correlation
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 0 | 133
   - 19.5 | 127
   - 40 | 149
   - 50 | 162

8. **Oleszek-Kudlak et al. 2004**
   - Generator column-GC/ECD
   - \( t/°C \) | \( S / g \cdot m^{-3} \)
   - 25 | 93.7
   - 35 | 108.0
   - 45 | 122.7
   - 55 | 130.1

\( \Delta H_{\text{sol}} = 10.49 \text{ kJ/mol} \)
FIGURE 6.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.2
Reported vapor pressures of 1,2-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \log (T/K) \quad (4) \\
\ln (P/P_a) &= (1 - T/T_o) \exp[\sum A_i T_i] \quad (5) - \text{Cox eq.}
\end{align*}
\]

1.

<table>
<thead>
<tr>
<th>Summary of Lit. Data</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>McDonald et al. 1959</th>
<th>Grayson &amp; Fosbraey 1982</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
</tr>
<tr>
<td>20</td>
<td>133.3</td>
<td>87.02</td>
<td>5010</td>
</tr>
<tr>
<td>46</td>
<td>666.6</td>
<td>97.66</td>
<td>7605</td>
</tr>
<tr>
<td>59.1</td>
<td>1333</td>
<td>104.94</td>
<td>10114</td>
</tr>
<tr>
<td>73.4</td>
<td>2666</td>
<td>118.32</td>
<td>16500</td>
</tr>
<tr>
<td>89.4</td>
<td>5333</td>
<td>147.6</td>
<td>42066</td>
</tr>
<tr>
<td>99.5</td>
<td>7999</td>
<td>164.65</td>
<td>67661</td>
</tr>
<tr>
<td>112.9</td>
<td>13332</td>
<td>180.48</td>
<td>101325</td>
</tr>
<tr>
<td>133.4</td>
<td>26664</td>
<td></td>
<td></td>
</tr>
<tr>
<td>155.8</td>
<td>53329</td>
<td></td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>101325</td>
<td></td>
<td>eq. 2</td>
</tr>
<tr>
<td></td>
<td>7.32585</td>
<td>A</td>
<td>7.07028</td>
</tr>
<tr>
<td>mp°C</td>
<td>–17.6</td>
<td>B</td>
<td>1824.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
© 2006 by Taylor & Francis Group, LLC
### TABLE 6.1.1.2.2 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>−14.2</td>
<td>7.73</td>
<td>−16.65</td>
<td>7.056</td>
<td>90.193</td>
<td>5729</td>
<td>263.15</td>
<td>12.9</td>
</tr>
<tr>
<td>−5.0</td>
<td>14.7</td>
<td>−16.65</td>
<td>7.042</td>
<td>99.529</td>
<td>8333</td>
<td>273.15</td>
<td>30.1</td>
</tr>
<tr>
<td>10</td>
<td>56.1</td>
<td>−9.75</td>
<td>13.175</td>
<td>99.53</td>
<td>8335</td>
<td>283.15</td>
<td>65.4</td>
</tr>
<tr>
<td>25</td>
<td>164</td>
<td>−9.75</td>
<td>13.195</td>
<td>107.0</td>
<td>11074</td>
<td>303.15</td>
<td>133.8</td>
</tr>
<tr>
<td>40</td>
<td>448</td>
<td>0.30</td>
<td>30.815</td>
<td>113.265</td>
<td>13917</td>
<td>313.15</td>
<td>259.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10.32</td>
<td>67.088</td>
<td>118.61</td>
<td>16800</td>
<td>323.15</td>
<td>477.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20.35</td>
<td>137.3</td>
<td>118.61</td>
<td>16799</td>
<td>333.15</td>
<td>843.3</td>
</tr>
<tr>
<td>ΔHv/(kJ mol⁻¹) = 51.2</td>
<td>30.28</td>
<td>264.39</td>
<td>124.14</td>
<td>20290</td>
<td>333.15</td>
<td>1430</td>
<td></td>
</tr>
<tr>
<td></td>
<td>40.24</td>
<td>485.45</td>
<td>129.935</td>
<td>24569</td>
<td>343.25</td>
<td>2338</td>
<td></td>
</tr>
<tr>
<td></td>
<td>50.15</td>
<td>848.67</td>
<td>135.547</td>
<td>29394</td>
<td>353.15</td>
<td>5681</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60.15</td>
<td>1400.7</td>
<td>141.024</td>
<td>34818</td>
<td>363.15</td>
<td>8491</td>
<td></td>
</tr>
<tr>
<td></td>
<td>70.05</td>
<td>2313.0</td>
<td>146.292</td>
<td>40757</td>
<td>373.15</td>
<td>12380</td>
<td></td>
</tr>
<tr>
<td></td>
<td>70.05</td>
<td>2318.6</td>
<td>151.657</td>
<td>47825</td>
<td>383.15</td>
<td>17640</td>
<td></td>
</tr>
<tr>
<td></td>
<td>80.02</td>
<td>3660.3</td>
<td>160.102</td>
<td>60273</td>
<td>393.15</td>
<td>45370</td>
<td></td>
</tr>
<tr>
<td></td>
<td>80.03</td>
<td>3661.2</td>
<td>168.184</td>
<td>74765</td>
<td>403.15</td>
<td>78370</td>
<td></td>
</tr>
<tr>
<td></td>
<td>88.75</td>
<td>5428.4</td>
<td>176.912</td>
<td>93403</td>
<td>413.15</td>
<td>10080</td>
<td></td>
</tr>
<tr>
<td></td>
<td>88.75</td>
<td>54284</td>
<td>178.845</td>
<td>97970</td>
<td>423.15</td>
<td>12380</td>
<td></td>
</tr>
<tr>
<td></td>
<td>89.94</td>
<td>5606.9</td>
<td>181.633</td>
<td>104893</td>
<td>433.15</td>
<td>17640</td>
<td></td>
</tr>
<tr>
<td></td>
<td>89.94</td>
<td>5601.2</td>
<td>184.102</td>
<td>12810</td>
<td>443.15</td>
<td>45370</td>
<td></td>
</tr>
<tr>
<td></td>
<td>98.79</td>
<td>8102.5</td>
<td>bp/°C</td>
<td>180.190</td>
<td>453.15</td>
<td>78370</td>
<td></td>
</tr>
<tr>
<td></td>
<td>98.79</td>
<td>8104.0</td>
<td>eq. 3</td>
<td>P/kPa</td>
<td>463.15</td>
<td>12810</td>
<td></td>
</tr>
<tr>
<td></td>
<td>108.76</td>
<td>11826</td>
<td>eq. 5</td>
<td>A 6.016161</td>
<td>473.15</td>
<td>90.193</td>
<td>5729</td>
</tr>
<tr>
<td></td>
<td>118.8</td>
<td>16870</td>
<td>A 6.16161</td>
<td>483.15</td>
<td>263.15</td>
<td>12.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>128.19</td>
<td>23583</td>
<td>B 1612.27</td>
<td>493.15</td>
<td>273.15</td>
<td>30.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>138.83</td>
<td>32396</td>
<td>C −64.447</td>
<td>493.15</td>
<td>283.15</td>
<td>65.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>148.91</td>
<td>43690</td>
<td>−64.447</td>
<td>503.15</td>
<td>293.15</td>
<td>133.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>eq. 3a</td>
<td>P/Pa</td>
<td>10⁻²A₂</td>
<td>6.0235167</td>
<td>513.15</td>
<td>303.15</td>
<td>259.1</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>21.5929</td>
<td>10⁻²A₂</td>
<td>1612.27</td>
<td>523.15</td>
<td>313.15</td>
<td>477.9</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>4053.86</td>
<td>10⁻²A₂</td>
<td>16870</td>
<td>533.15</td>
<td>323.15</td>
<td>843.3</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>−50.2358</td>
<td>10⁻²A₂</td>
<td>16925</td>
<td>543.15</td>
<td>333.15</td>
<td>1430</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
TABLE 6.1.1.2.3
Reported Henry’s law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2-dichlorobenzene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log ( K_{OW} )</th>
<th>( \log K_{OA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/°C</td>
<td>H/(Pa m³/mol)</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>10</td>
<td>165</td>
<td>5</td>
</tr>
<tr>
<td>15</td>
<td>145</td>
<td>15</td>
</tr>
<tr>
<td>20</td>
<td>170</td>
<td>25</td>
</tr>
<tr>
<td>20</td>
<td>159</td>
<td>35</td>
</tr>
<tr>
<td>30</td>
<td>240</td>
<td>45</td>
</tr>
</tbody>
</table>

\[
\ln H = A - B(T/K) \quad \Delta H/(kJ mol^{-1}) = -17.8 \quad \Delta H_{OA}/(kJ mol^{-1}) = 49.3 \quad \Delta H_{OA}/(kJ mol^{-1}) = 57.02
\]

\[
\log K_{OW} = A - \Delta H/2.303RT \quad \log K_{OA} = A + B/RT \quad \log K_{OA} = A + B/2.303RT
\]

© 2006 by Taylor & Francis Group, LLC
FIGURE 6.1.1.2.3 Logarithm of Henry's law constant, $K_{OW}$, and $K_{OA}$ versus reciprocal temperature for 1,2-dichlorobenzene.
6.1.1.3 1,3-Dichlorobenzene

Common Name: 1,3-Dichlorobenzene
Synonym: m-dichlorobenzene
Chemical Name: 1,3-dichlorobenzene
CAS Registry No: 541-73-1
Molecular Formula: C₆H₄Cl₂
Molecular Weight: 147.002
Melting Point (°C):
-24.8 (Lide 2003)
Boiling Point (°C):
173 (Lide 2003)
Density (g/cm³ at 20°C):
1.2884 (Dreisbach 1955; Weast 1972–73; Horvath 1982; Lide 2003)
Molar Volume (cm³/mol):
114.1 (20°C, calculated-density)
137.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
12.64 (Weast 1972–73)
Enthalpy of Fusion, \( \Delta H_f \) (kJ/mol):
50.63 (Pirsch 1956)
51.46 (Yalkowsky 1979)
51.05 (Yalkowsky & Valvani 1980)
Entropy of Fusion, \( \Delta S_f \) (J/mol K):
Fugacity Ratio at 25°C, F:
1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
123* (volumetric, measured range 20–60°C, Klemenc & Löw 1930)
123.5 (Ginnings et al. 1939)
124 (Landolt-Börnstein 1951)
101.26* (shake flask-UV, measured range 10–35°C, Vesala 1973)
102.9 (shake flask-UV, Vesala 1974)
119.5 (shake flask-UV, Yalkowsky et al. 1979)
131 (shake flask-LSC-14C, Veith et al. 1980)
144*, 149 (23.5°C, elution chromatography, measured range 10–30°C, Schwarz 1980)
111, 89, 113 (20°C, quoted, UV, elution chromatography, average exptl. value, Schwarz & Miller 1980)
133.5 (shake flask-LSC, Banerjee et al. 1980)
68.6 (shake flask-GC, Könemann 1981)
124 (recommended, Horvath 1982)
124.5 (generator column-GC/ECD, Miller et al. 1984, 1985)
143 (shake flask-HPLC, Banerjee 1984)
106* (recommended, temp range 10–60°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

\[ S/(g/kg) = 27.6827 - 2.61597 \times 10^{-1}(T/K) + 8.19706 \times 10^{-4}(T/K)^2 - 8.4698 \times 10^{-7}(T/K)^3, \] temp range 283–333 K
(regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

110 (Dean 1985)
111 (20°C, Riddick et al. 1986)
130 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
123; 138 (quoted lit.; shake flask-GC, Boyd et al. 1998)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (12.1°C, summary of literature data, Stull 1947)
log (P/mmHg) = 7.30364 – 1782.4/(C + t/°C) (Antoine eq., Dreisbach & Martin 1949)
7605* (90.7°C, ebulliometry, measured range 90.72–173.0°C, Dreisbach & Shrader 1949)
252 (extrapolated by formula., Dreisbach 1955)
log (P/mmHg) = 6.88045 – 1496.2/(201.0 + t/°C); temp range 75–240°C (Antoine eq., Dreisbach 1955)
307 (extrapolated, Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 10446.8/(T/K)] + 8.017555; temp range 12.1–173°C (Antoine eq., Weast 1972–73)
266 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.17083 – 1611.2/(213.817 + t/°C); temp range 90.7–173°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
179.3 (gas saturation, interpolated from reported graph, Rordorf 1985)
265 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.0401 – 1607.05/(213.38 + t/°C); temp range 91–173°C (Antoine eq., Dean 1985, 1992)
243 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.00535 – 1496.2/(–72.15 + T/K); temp range 348–513 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
236 (supercooled liquid P L, GC-Kovás retention indices correlation; Spieksma et al. 1994)
190.4* (20.39°C, static-pressure gauge, measured range –25 to 159°C, Polednicek et al. 1996)
ln [(P/Pa)/4.85] = [1 – (T/K)/248.39]·exp{3.366439 – 8.3811530 × 10 –4·(T/K) + 5.9337577 × 10–7(T/K)2}; temp range 250–448 K (Cox eq., recommended, Roháč et al. 1999)
log (P/Pa) = 21.6433 – 4031.27/(T/K) – 47.5846; temp range 249–432 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
log (P/mmHg) = 3.2904 – 2.5839 × 106/(T/K) + 3.893·log (T/K) – 9.5398 × 10 –3·(T/K) + 4.6397 × 10–6·(T/K)2, temp range 248–684 K, (Yaws 1994)
5731* (84.353°C, comparative ebulliometry, measured range 84.353–175.207°C, Roháč et al. 1998)
185.0* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)
In [(P/Pa)/4.85] = [1 – (T/K)/248.39]·exp{3.366439 – 8.3811530 × 10 –4·(T/K) + 5.9337577 × 10–7(T/K)2}; temp range 250–448 K (Cox eq., recommended, Roháč et al. 1999)
log (P/Pa) = 21.6433 – 4031.27/(T/K) – 47.5846; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

472 (calculated as 1/K AW, Cw/C A, reported as exptl., Hine & Mookerjee 1975; selected exptl., Nirmalan-khandan & Speece 1988a)
375 (calculated-bond contribution, Hine & Mookerjee 1975)
182 (20°C, batch air stripping-GC, Oliver 1985)
267 (gas stripping-GC, Warner et al. 1987)
289* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
ln [H/(atm·m³/mol)] = 2.882 – 2564/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
328 (computer value, Yaws et al. 1991)
216 (20°C, equilibrium gas stripping-GC, Hovorka & Dohnal 1997)
269 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)
288 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K AW = 2.436 – 986/(T/K) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K OW at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.55 (Hansch et al. 1968)
3.38 (Leo et al. 1971; Hansch & Leo 1979)
3.57, 3.55 (calculated-fragment constants, Rekker 1977)
3.60 (shake flask-GC, Könemann et al. 1979)
3.62 (HPLC-κ′ correlation, Könemann et al. 1979)
3.44 (shake flask-LSC, Banerjee et al. 1980)
3.44 (shake flask-LSC, Veith et al. 1980; Oliver & Niimi 1983)
3.95 (HPLC-RT correlation, Veith et al. 1980)
3.53 (shake flask-GC, Watarai et al. 1982)
3.46 (shake flask-HPLC, Hammers et al. 1982)
3.38–3.62, 3.52 (range, mean, shake flask method, Eadsforth & Moser 1983)
3.62–3.95, 3.73 (range, mean, HPLC method, Eadsforth & Moser 1983)
3.48 (generator column-HPLC/UV, Wasik et al. 1983)
3.48 (generator column-GC/ECD, Miller et al. 1984; 1985)
3.57 (HPLC-RV correlation, Garst 1984)
3.60 (Hansch & Leo 1985)
3.55* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
3.50 (shake flask-GC, Pereira et al. 1988)
3.525 (slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
3.52 (recommended, Sangster 1993)
3.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated
* are compiled at the end of this section:

4.36 (calculated-$S_{oc}$ and vapor pressure, Abraham et al. 2001)
4.27* (20°C, HPLC-κ′ correlation, measured range 10–50°C, Su et al. 2002)

\[
\log K_{OA} = 57020/(2.303·RT) – 5.856; \text{ temp range } 10–50°C (\text{HPLC-κ′ correlation, Su et al. 2002})
\]

Bioconcentration Factor, log BCF:

1.82 (bluegill sunfish, Veith et al. 1979b; 1980)
1.82 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
2.86 (microorganisms-water, Mabey et al. 1982)
2.57–2.68 mean 2.62; 2.74–2.96 mean 2.87 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
3.70–4.02 (rainbow trout, lipid base, Oliver & Niimi 1983)
2.62–2.87 (fish, Oliver 1984)
1.99 (fathead minnow, flowing water, Carlson & Kosian 1987)
3.77, 3.78, 3.83, 3.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
3.60, 3.86, 3.25, 3.40 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
1.82; 2.62, 2.87 (Lepomis macrochirus; Oncorhynchus mykiss, quoted lit., flow through conditions, Devillers et al. 1996)
3.78 (Poecilia reticulata, quoted lit., static and semi-static conditions, Devillers et al. 1996)
2.62, 3.70; 2.553, 2.305 (quoted: whole fish, lipid content; calculated-QSPR-MCI $\chi$, $K_{OW}$, Lu et al. 1999)
3.79; 3.75 (Oncorhynchus mykiss, wet wt. basis: quoted exprtl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log $K_{OC}$:

4.50; 4.10 (field data of sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
2.14 (soil, Lee et al. 1989)
2.48 (soil, calculated-QSAR-MCI $\chi$, Sabljic et al. 1995)
2.43, 2.58, 2.88 (RP-HPLC-κ′ correlation on three different stationary phases, Szabo et al. 1995)
2.60, 2.60 (RP-HPLC-κ′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
3.47 ± 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
2.49, 2.53 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
Sorption Partition Coefficient, log $K_{OM}$:

- 2.23 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
- 3.88 (micelle-water, Valsaraj & Thibodeaux 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:

Volatilization: estimated $t_\text{½} = 4.1$ h from a model river of 1 m depth with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);
- $k = 1.9 \times 10^{-4}$ h$^{-1}$ with $H_2O_2$ at 25°C in F-113 solution and with $HO^-$ in the gas (Dilling et al. 1988);
- pseudo-first-order direct photolysis $k(\text{exptl}) = (0.008. \pm 0.001)$ min$^{-1}$ with $t_{\text{½}} = (92.3 \pm 6.4)$ min in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_O$ or as indicated, *data at other temperatures see reference:
- $k_{OH} \approx 3.0 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
- $k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k << 1$ M$^{-1}$ h$^{-1}$ for RO$_2$ radical (Mabey et al. 1982)
- $k_{OH} = (7.2 \pm 0.2) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

Hydrolysis: not environmentally significant (Mabey et al. 1982)

- base rate constant $k < 0.9$ M$^{-1}$ h$^{-1}$ at 25°C with a calculated $t_{\text{½}} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)
- first-order $t_{\text{½}} > 879$ yr, based on rate constant $k < 0.9$ M$^{-1}$ h$^{-1}$ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation: significant degradation in an aerobic environment with rate constant $k = 0.05$ d$^{-1}$ (Tabak et al. 1981; Mills et al. 1982);

Biotransformation: $k = 1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
  $t_{\text{½}} = 200.6–2006$ h, based on photooxidation half-life in air (Howard et al. 1991).
- Surface Water: $t_{\text{½}} = 0.9$–50 d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1983; selected, Howard 1989)
  $t_{\text{½}} = 50$–3420 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation: significant degradation in an aerobic environment with rate constant $k = 0.05$ d$^{-1}$ (Tabak et al. 1981; Mills et al. 1982);

nearly 100% removed by an apparent combination of biodegradation and stripping in a continuous flow activated sludge system (Kincannon et al. 1983; selected, Howard 1989)

$Me$ (aq. aerobic) $= 672–4320$ h, estimated from unacclimated soil grab sample data; $t_{\text{½}}(\text{aq. anaerobic}) = 2688–17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Groundwater: \( t_{1/2} = 1 \text{ yr} \) estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

\( t_{1/2} = 1334–8640 \text{ h} \), based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: \( t_{1/2} = 672–4320 \text{ h} \), based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: \( t_{1/2} < 1 \text{ d} \) in bluegill sunfish (Veith et al. 1980; Barrows et al. 1980)

\( t_{1/2} < 5 \text{ d} \) in worm at 8°C (Oliver 1987a);
biochemical half-lives, \( t_{1/2} < 1 \text{ d} \) in trout muscle, \( t_{1/2} < 1 \text{ d} \) in sunfish, and \( t_{1/2} < 1 \text{ d} \) in guppy for dichlorobenzenes (Niimi 1987).

### TABLE 6.1.1.3.1
Reported aqueous solubilities of 1,3-dichlorobenzene at various temperatures

1.

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Klemenc &amp; Löw 1930</th>
<th>Vesala 1973</th>
<th>Schwarz &amp; Miller 1980</th>
<th>Horvath &amp; Getzen 1985</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>volumetric method</td>
<td>shake flask-UV spec.</td>
<td>elution chromatography</td>
<td>recommended values</td>
</tr>
<tr>
<td>20</td>
<td>111</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>25</td>
<td>123</td>
<td>15.2</td>
<td>20</td>
<td>15</td>
</tr>
<tr>
<td>30</td>
<td>140</td>
<td>19.6</td>
<td>30</td>
<td>20</td>
</tr>
<tr>
<td>35</td>
<td>150</td>
<td>25.1</td>
<td>30</td>
<td>25</td>
</tr>
<tr>
<td>40</td>
<td>167</td>
<td>30.0</td>
<td>10</td>
<td>30</td>
</tr>
<tr>
<td>45</td>
<td>177</td>
<td>35.0</td>
<td>20</td>
<td>35</td>
</tr>
<tr>
<td>55</td>
<td>196</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>201</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Ma et al. 2001</th>
<th>Finizio &amp; Di Guardo 2001</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-GC</td>
<td>RP-HPLC-k’ correlation</td>
</tr>
<tr>
<td>5</td>
<td>114</td>
<td>5</td>
</tr>
<tr>
<td>15</td>
<td>108</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>126</td>
<td>25</td>
</tr>
<tr>
<td>35</td>
<td>134</td>
<td>35</td>
</tr>
<tr>
<td>45</td>
<td>141</td>
<td>45</td>
</tr>
</tbody>
</table>
FIGURE 6.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.2
Reported vapor pressures of 1,3-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.1</td>
<td>133.3</td>
<td>90.72</td>
<td>7605</td>
<td>-23.55</td>
<td>5.459</td>
<td>84.353</td>
<td>5731</td>
</tr>
<tr>
<td>39</td>
<td>666.6</td>
<td>98.05</td>
<td>10114</td>
<td>-19.57</td>
<td>7.973</td>
<td>93.65</td>
<td>8343</td>
</tr>
<tr>
<td>52.9</td>
<td>1333</td>
<td>111.49</td>
<td>16500</td>
<td>-19.57</td>
<td>7.973</td>
<td>97.99</td>
<td>11076</td>
</tr>
<tr>
<td>66.2</td>
<td>2666</td>
<td>140.49</td>
<td>42060</td>
<td>-9.7</td>
<td>19.355</td>
<td>107.17</td>
<td>13922</td>
</tr>
<tr>
<td>82</td>
<td>5333</td>
<td>157.37</td>
<td>67660</td>
<td>0.3</td>
<td>44.155</td>
<td>112.43</td>
<td>16799</td>
</tr>
<tr>
<td>92.2</td>
<td>7999</td>
<td>173.0</td>
<td>101325</td>
<td>10.34</td>
<td>94.451</td>
<td>117.89</td>
<td>20292</td>
</tr>
<tr>
<td>105</td>
<td>13332</td>
<td>173.0</td>
<td>101325</td>
<td>10.35</td>
<td>9.459</td>
<td>117.89</td>
<td>20291</td>
</tr>
<tr>
<td>125.9</td>
<td>26664</td>
<td>bp/°C</td>
<td>-24.76</td>
<td>20.39</td>
<td>190.4</td>
<td>123.625</td>
<td>24569</td>
</tr>
<tr>
<td>149</td>
<td>53329</td>
<td>bp/°C</td>
<td>173.0</td>
<td>30.28</td>
<td>360.02</td>
<td>129.141</td>
<td>29396</td>
</tr>
<tr>
<td>173</td>
<td>101325</td>
<td>eq. 2</td>
<td>P/mmHg</td>
<td>40.26</td>
<td>652.82</td>
<td>134.535</td>
<td>34819</td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Polednicek et al. 1996</th>
<th>Roháč et al. 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>summary of literature data</td>
<td>ebulliometry</td>
<td>static method-pressure gauge</td>
<td>comparative ebulliometry</td>
</tr>
<tr>
<td>$t/\degree C$</td>
<td>$P/\text{Pa}$</td>
<td>$t/\degree C$</td>
<td>$P/\text{Pa}$</td>
</tr>
<tr>
<td>89.94</td>
<td>7042.6</td>
<td>174.92</td>
<td>105933</td>
</tr>
<tr>
<td>89.94</td>
<td>7049.0</td>
<td>175.207</td>
<td>106716</td>
</tr>
<tr>
<td>98.86</td>
<td>10180</td>
<td></td>
<td></td>
</tr>
<tr>
<td>108.83</td>
<td>14713</td>
<td>173.095</td>
<td></td>
</tr>
<tr>
<td>118.87</td>
<td>20859</td>
<td></td>
<td></td>
</tr>
<tr>
<td>128.93</td>
<td>28986</td>
<td>eq. 3</td>
<td>P/kPa</td>
</tr>
<tr>
<td>138.94</td>
<td>39411</td>
<td>A</td>
<td>6.16151</td>
</tr>
<tr>
<td>149.05</td>
<td>52842</td>
<td>B</td>
<td>1595.19</td>
</tr>
<tr>
<td>159.06</td>
<td>69604</td>
<td>C</td>
<td>–62.398</td>
</tr>
<tr>
<td>eq. 3a</td>
<td></td>
<td>P/Pa</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>21.6433</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>4031.27</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>–47.5846</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>Roháč et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>recommended</td>
</tr>
<tr>
<td>$T/\text{K}$</td>
</tr>
<tr>
<td>253.15</td>
</tr>
<tr>
<td>263.15</td>
</tr>
<tr>
<td>273.15</td>
</tr>
<tr>
<td>283.15</td>
</tr>
<tr>
<td>283.15</td>
</tr>
<tr>
<td>303.15</td>
</tr>
<tr>
<td>313.15</td>
</tr>
<tr>
<td>232.15</td>
</tr>
<tr>
<td>333.15</td>
</tr>
<tr>
<td>343.25</td>
</tr>
<tr>
<td>353.15</td>
</tr>
<tr>
<td>363.15</td>
</tr>
<tr>
<td>373.15</td>
</tr>
<tr>
<td>383.15</td>
</tr>
<tr>
<td>393.15</td>
</tr>
<tr>
<td>403.15</td>
</tr>
<tr>
<td>413.15</td>
</tr>
<tr>
<td>423.15</td>
</tr>
<tr>
<td>433.15</td>
</tr>
<tr>
<td>443.15</td>
</tr>
<tr>
<td>453.15</td>
</tr>
<tr>
<td>Cox eq.</td>
</tr>
<tr>
<td>eq. 5</td>
</tr>
<tr>
<td>$A_0$</td>
</tr>
<tr>
<td>$10^{-6}A_i$</td>
</tr>
</tbody>
</table>
TABLE 6.1.1.3.2 (Continued)

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^{-2}A_2)</td>
<td>5.9337577</td>
</tr>
<tr>
<td>(T/K)</td>
<td>248.39</td>
</tr>
<tr>
<td>(P_0/Pa)</td>
<td>4.85</td>
</tr>
<tr>
<td>bp/K</td>
<td>446.25</td>
</tr>
</tbody>
</table>

T/K \(=250-448\) K

FIGURE 6.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,3-dichlorobenzene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log (K_{OW})</th>
<th>log (K_{OA})</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ashworth et al. 2988</strong></td>
<td><strong>Opperhuzen et al. 1988</strong></td>
<td><strong>Su et al. 2002</strong></td>
</tr>
<tr>
<td>EPICS-GC</td>
<td>shake flask-GC/ECD</td>
<td>GC-RT correlation</td>
</tr>
<tr>
<td>t/°C</td>
<td>(H/(Pa \cdot m^3/mol))</td>
<td>t/°C</td>
</tr>
<tr>
<td>10</td>
<td>224</td>
<td>13</td>
</tr>
<tr>
<td>15</td>
<td>234</td>
<td>19</td>
</tr>
<tr>
<td>20</td>
<td>298</td>
<td>28</td>
</tr>
<tr>
<td>20</td>
<td>289</td>
<td>33</td>
</tr>
<tr>
<td>30</td>
<td>428</td>
<td>50</td>
</tr>
</tbody>
</table>

\(\Delta H/(kJ \cdot mol^{-1}) = -15.0\).

\(\log K_{OA} = A + B/2.303RT\)

A 57020

© 2006 by Taylor & Francis Group, LLC
FIGURE 6.1.1.3.3 Logarithm of Henry’s law constant, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,3-dichlorobenzene.
### 1,4-Dichlorobenzene

- **Common Name:** 1,4-Dichlorobenzene
- **Synonym:** \( p \)-dichlorobenzene, paradichlorobenzene
- **Chemical Name:** 1,4-dichlorobenzene
- **CAS Registry No:** 106-46-7
- **Molecular Formula:** \( \text{C}_6\text{H}_4\text{Cl}_2 \)
- **Molecular Weight:** 147.002
- **Melting Point (°C):** 53.09 (Lide 2003)
- **Boiling Point (°C):** 174 (Lide 2003)
- **Density (g/cm\(^3\) at 20°C):** 1.2457 (Dreisbach 1955; Weast 1972–73; Horvath 1982)
- **Molar Volume (cm\(^3\)/mol):**
  - 118.0 (20°C, calculated-density)
  - 137.8 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):**
  - 18.72 (Dreisbach 1955)
  - 17.882 (Weast 1972–73)
  - 18.16, 18.70 (Wauchope & Getzen 1972)
  - 18.20 (Tsonopoulos & Prausnitz 1971; Dean 1985)
  - 19.0 (Miller et al. 1984)
  - 17.153 (Ruelle et al. 1993)
- **Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):**
  - 55.65 (Tsonopoulos & Prausnitz 1971)
  - 54.81 (Weast 1976–77; Amidon & Williams 1982; Yalkowsky 1979)
  - 56.07 (Yalkowsky & Valvani 1980)
  - 58.16 (Miller et al. 1984)
- **Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \), F: 0.53 (mp at 53.09°C)**
- **Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**
  - 79.1* (volumetric method, measured range 20–60°C, Klemenc & Löw 1930)
  - 77 (30°C, shake flask-interferometer, Gross & Saylor 1930)
  - < 500 (residue-volume method, Booth & Everson 1948)
  - 76 (shake flask-UV, Andrew & Keefer 1950)
  - 89.8 (Landolt-Börnstein 1951)
  - 83.4* (24.6°C, shake flask-UV, measured 22.2–73.4°C, Wauchope & Getzen 1972)
  - 85.5 (shake flask-UV, Vesala 1974)
  - 56.9 (20°C, shake flask-GC/ECD, Chiou & Freed 1977)
  - 34 (shake flask-GC, Jones et al. 1977/1978)
  - 87.2 (shake flask-GC, Aquan-Yuen et al. 1979)
  - 90.6 (shake flask-UV, Yalkowsky et al. 1979)
  - 73.7 (shake flask-LSC, Veith et al. 1980)
  - 73.8 (shake flask-LSC, Banerjee et al. 1980)
  - 48.7 (shake flask-GC, Könemann 1981)
  - 73, 137 (shake flask-GC, solid, supercooled liquid, Chiou et al. 1982)
90.0  (recommended, Horvath 1982)
25  (calculated-UNIFAC activity coefficients, Arbuckle 1983)
175  (calculated-HPLC-k', converted from reported \( \gamma_W \), Hafkenscheid & Tomlinson 1983a)
154  (30°C, shake flask-GC, McNally & Grob 1983)
30.9  (generator column-GC, Miller et al. 1984, 1985)
65.3  (shake flask-HPLC, Banerjee 1984)
158  (30°C, shake flask-GC, McNally & Grob 1984)
82.9*  (recommended, temp range 10–75°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

\[
S/(g/kg) = 13.974 - 8.5829 \times 10^{-2} \times (T/K) + 1.3365 \times 10^{-4} \times (T/K)^2; \text{ temp range 328–348 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)}
\]

100  (Dean 1985)
141  (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
81.4* ± 1.5  (shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
42.0  (shake flask-GC, Boyd et al. 1998)

\[
\ln x = -4.178 - 2186.7/(T/K); \text{ temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)}
\]

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

\[
1333* \quad (54.8°C, \text{summary of literature data, temp range 54.8–173.9°C, Stull 1947})
\]

\[
\log (P/mmHg) = 7.30697 - 1788.7/(230 + t/°C) \quad (\text{Antoine eq., Dreisbach & Martin 1949})
\]

\[
7605* \quad (92.0°C, \text{ebulliometry, measured range 92.0–174.12°C, Dreisbach & Shrader 1949})
\]

\[
235 \quad (\text{calculated by formula., Dreisbach 1955; quoted, Hine & Mookerjee 1975; Riddick et al. 1986; Howard 1989})
\]

\[
\log (P/mmHg) = 6.89797 - 1507.3/(201.0 + t/°C); \text{ temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)}
\]

\[
8514* \quad (94.8°C, \text{ebulliometry, measured range 94.8–174.04°C, McDonald et al. 1959})
\]

\[
93.33* \quad (20.4°C, \alpha-p\text{-dichlorobenzene, manometry, measured range 20.4–39.6°C, Walsh & Smith 1961})
\]

\[
402.6* \quad (37.9°C, \beta-p\text{-dichlorobenzene, manometry, measured range 37.9–52.5°C, Walsh & Smith 1961})
\]

\[
90.2 \quad (\text{solid vapor pressure, extrapolated, Antoine eq., Weast 1972–73})
\]

\[
\log (P/mmHg) = [-0.2185 \times 17260.5/(T/K)] + 12.4800; \text{ temp range 30–50°C, (Antoine eq., Weast 1972–73)}
\]

\[
\log (P/mmHg) = [-0.2185 \times 10611.0/(T/K)] + 8.073632; \text{ temp range 54.8–173.9°C (Antoine eq., Weast 1972–73)}
\]

\[
137.2* \quad (\text{diaphragm pressure gauge, measured range: 0–20°C, De Kruif et al. 1981})
\]

\[
128 \quad (\text{extrapolated-Antoine eq., Boublik et al. 1984})
\]

\[
\log (P/mmHg) = 5.94201 – 1668.235/(186.212 + t/°C); \text{ temp range 164.7–237.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984})
\]

\[
158* \quad (\text{gas saturation-GC, measured range 20–100°C, Rordorf 1985})
\]

\[
243 \quad (\text{extrapolated-Antoine eq., Dean 1985})
\]

\[
\log (P/mmHg) = 7.0208 – 1507.3/(201.0 + t/°C); \text{ temp range 95–174°C (Antoine eq., Dean 1985, 1992})
\]

\[
86.7 \quad (20°C, \text{gas saturation, Chiou & Shoup 1985})
\]

\[
134 \quad (\text{interpolated-Antoine eq.-I, Stephenson & Malanowski 1987})
\]

\[
\log (P/kPa) = 10.472 – 3382.9/(T/K); \text{ temp range 293–313 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987})
\]

\[
\log (P/kPa) = 10.181 – 3290.4/(T/K); \text{ temp range 310–336 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987})
\]

\[
\log (P/kPa) = 6.12695 – 1578.51/(-64.22 + T/K); \text{ temp range 341–448 K (liquid, Antoine eq., Stephenson & Malanowski 1987})
\]

\[
133* \quad (\text{gas saturation-GC, measured range −15 to 40°C, Liu & Dickhut 1994})
\]

\[
216; 257 \quad (\text{supercooled liquid P}_s, \text{GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994})
\]

\[
\log (P/mmHg) = 36.2276 – 3.6756 \times 10^9/(T/K) - 9.6308 \times 10^9/(T/K)^2 + 1.9905 \times 10^{-6} \times (T/K)^3; \text{ temp range 326–685 K (vapor pressure eq., Yaw et al. 1994})
\]

\[
135* \quad (25°C; \text{pressure gauge measurement; interpolated from reported Antoine eq., Polednicek et al. 1996})
\]

\[
\ln (P_s/Pa) = 28.4986 – 6272.86/(T/K) – 32.2741; \text{ temp range 273–323 K (Antoine eq. from exptl. data, pressure gauge measurement, solid, Polednicek et al. 1996})
\]

\[
\ln (P_{s}/Pa) = 21.0472 – 3665.96/(T/K) – 62.3849; \text{ temp range 333–442 K (Antoine eq. from exptl. data, pressure gauge measurement, liquid, Polednicek et al. 1996})
\]
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

5729* (85.139°C, comparative ebulliometry, measured range 85.139–175.626°C, Roháč et al. 1998)
87.0* (20°C, recommended, summary of literature data, temp range 273.15–453.15 K, Roháč et al. 1999)
\[ \ln \left( \frac{PS/Pa}{1280} \right) = \left[ 1 - \frac{T}{326.3K} \right] \cdot \exp \left\{ 3.251427 - 2.853921 \times 10^{-4} \cdot \frac{T}{K} \right\} \]; temp range 273–323 K (Cox eq., solid, recommended, Roháč et al. 1999)
\[ \ln \left( \frac{PL/Pa}{1280} \right) = \left[ 1 - \frac{T}{326.3K} \right] \cdot \exp \left\{ 3.100023 - 1.0557743 \times 10^{-3} \cdot \frac{T}{K} + 7.816354 \times 10^{-7} \cdot \frac{T}{K^2} \right\} \]; temp range 328–449 K (Cox eq., liquid, recommended, Roháč et al. 1999)
\log (P/Pa) = 11.63209 - 2829.32/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
330 (equilibrium cell-GC, concentration ratio, Leighton & Calo 1981)
240 (gas stripping-GC, Mackay & Shiu 1981)
152 (20°C, gas stripping-GC, Oliver 1985)
276 (gas stripping-GC, Warner et al. 1987)
321* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
\ln \left( \frac{H}{(atm \cdot m^3/mol)} \right) = 3.373 - 2720/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
438 (computer value, Yaws et al. 1991)
244 (gas stripping-GC, Shiu & Mackay 1997)
188 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
275 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 2.649 - 1054/(T/K) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
3.39 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
3.57, 3.55 (calculated-fragment constants, Rekker 1977)
3.38 (Hansch & Leo 1979)
3.62, 3.39 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)
3.37, 3.78 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
3.37 (shake flask-LSC, Banerjee et al. 1980)
3.46 (HPLC-k’ correlation, Hammers et al. 1982)
3.52 (shake flask-GC, Watarai et al. 1982)
3.43 (HPLC-k’ correlation, Miyake & Terada 1982)
3.67, 3.90 (calculated-UNIFAC activity coefficients, Arbuckle 1983)
3.37 (generator column-HPLC/UV, Wasik et al. 1983)
3.38 (generator column-GC/ECD, Miller et al. 1984; 1985)
3.37 (HPLC-RV correlation, Garst 1984; Garst & Wilson 1984)
3.52 (Hansch & Leo 1985)
3.444 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
3.85–4.30, 4.0 (range, average: round robin work, shake flask or HPLC-k’ correlation, Kishi & Hashimoto 1989)
3.355 ± 0.053, 3.444 ± 0.001 (shake flask methods, interlaboratory studies, Brooke et al. 1990)
3.45 (recommended, Sangster 1993)
3.44 (recommended, Hansch et al. 1995)
3.23* ± 0.03 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
log K_{OW} = 0.2338 + 17100/(2.303·RT); temp range 5–45°C (van’t Hoff eq., Bahadur et al. 1997)
3.65 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.46 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
4.32* (20°C, HPLC-k’ correlation, measured range 10–50°C, Su et al. 2002)
log K_{OA} = 55590/(2.303-RT) – 5.556; temp range 10–50°C (HPLC-k’ correlation, Su et al. 2002)
Bioconcentration Factor, log BCF at 25°C or as indicated:

- 2.33 (rainbow trout, Neely et al. 1974)
- 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 1.78 (bluegill sunfish, Veith et al. 1979b, 1980)
- 1.78 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 3.26 (guppy, lipid basis, Königsmann & van Leeuwen 1980)
- 2.53–2.59 mean 2.57; 2.79–2.96 mean 2.86 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 3.64–3.96 (rainbow trout, lipid basis, Oliver & Niimi 1983)
- 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 1.78 (bluegill sunfish, Veith et al. 1979b, 1980)
- 1.78 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 3.26 (guppy, lipid basis, Königsmann & van Leeuwen 1980)
- 2.53–2.59 mean 2.57; 2.79–2.96 mean 2.86 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

Sorption Partition Coefficient, log K_{OC}:

- 2.59 (Kenaga 1980a)
- 2.29 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.18–3.44 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 4.80; 5.00 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
- 2.82; 2.45 (Apron soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium Southworth & Keller 1986)
- 5.30–5.60; 5.50 (Niagara River plume: range; average value; Oliver 1987b)
- 2.92; 2.91 (Aldrich humic acid, equilibrium dialysis; Aldrich and Fluka humic acid, Flory-Huggins model, Chin & Weber 1989)
- 2.43 (organic polymers in Huran River water, Chin et al. 1990)
- 2.88 (HPLC-k' correlation, Szabo et al. 1995)
- 2.60, 2.61 (RP-HPLC-k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.66, 2.57, 2.77 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
- 2.99–3.46 (three wetland soils, batch equilibrium-sorption isotherm-LSC, Lee et al. 2003)

Sorption Coefficient, log K_{OM}:

- 2.20 (Woodburn silt loam soil, organic matter 1.9%, equilibrium sorption isotherm, Chiou et al. 1983)
Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.3$ h from a model river of 1 m depth and with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982);

- rate constants: $k = 0.04 \text{ d}^{-1}$, $t_{1/2} = 18$ d in spring at 8–16°C, $k = 0.068 \text{ d}^{-1}$, $t_{1/2} = 10$ d in summer at 20–22°C, $k = 0.054 \text{ d}^{-1}$, $t_{1/2} = 13$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and
- $k = 0.066 \text{ d}^{-1}$, $t_{1/2} = 10.6$ d with HgCl$_2$, and $k = 0.063 \text{ d}^{-1}$, $t_{1/2} = 11$ d without HgCl$_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982)

- Direct photolysis unimportant (Zepp & Cline 1977; Zepp 1978);

- $t_{1/2} = 25$ d under sunlight in water (Mansour & Feicht 1994)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k = 9.63 \times 10^{-3} \text{ h}^{-1}$ in air (Ware & West 1977; selected, Mackay et al. 1985)
- $k_{OH} \approx 3.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
- $k = \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO$_2$ radical (Mabey et al. 1982)

- $k = \ll 3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 0.5 mM t-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

- $k_{OH} = (3.2 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

- $k_{OH} = 3.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{OH}(\text{calc}) = 4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

- $k_{OH}(\text{calc}) = 0.41 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{OH}(\text{obs}) = 0.32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

- $k_{HO-} = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

- $k_{OH}(\text{calc}) = 0.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982);

- base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

- first order $t_{1/2} > 879$ yr, based on rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation:

- $k = 1.09 \times 10^{-2} \text{ h}^{-1}$ degradation in water (Verschueren 1977)

- $t_{1/2}(\text{aq. aerobic}) = 672$–4320 h based on unacclimated aerobic screening test data (Canton et al. 1985) and aerobic soil grab sample data (Haider et al. 1981; Howard et al. 1991)

- $k = (5.0 – 5.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

- $k_{OH} = 0.32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993).

Biotransformation: $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 5.67 \text{ h}^{-1}$; $k_2 = 0.0264 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974; Neely 1979)

- $k_1 = 7.44 \text{ h}^{-1}$ (10°C, yellow perch, Neely et al. 1974; Neely 1979)

- $k_1 = 17.0 \text{ h}^{-1}$ (25°C, yellow perch, Neely et al. 1974; Neely 1979)

- $k_{k1} = 1800 \text{ d}^{-1}$; $k_2 = 1.00 \text{ d}^{-1}$ (guppy, Könemann & van Leeuwen 1980)

- $k_1 = 4.1 \text{ h}^{-1}$; $1/k_2 = 24$ h (guppy, quoted from Könemann & van Leeuwen 1980, Hawker & Connell 1985)

- $k_1 = 5.7 \text{ h}^{-1}$; $1/k_2 = 38$ h (rainbow trout, quoted from Neely et al. 1974, Hawker & Connell 1985)

- $k_1 = 97 \text{ d}^{-1}$ (fish, quoted, Opperhuizen 1986)

- $k_2 = 0.98 \text{ d}^{-1}$ (fish, calculated-KOW, Thomann 1989)

- $k_1 = 1.99 \text{ d}^{-1}$; $k_2 = 0.0$ (guppy, 12–31 d exposure experiments, Gobas et al. 1989)

- $k_1 = 1.99 \text{ d}^{-1}$ (fish, quoted, Connell & Hawker 1988)

- $k_1 = 291 \text{ d}^{-1}$, 4230 d$^{-1}$; $k_2 = 0.98 \text{ d}^{-1}$, 1.18 d$^{-1}$ (American flagfish: whole fish, fish lipid, Smith et al. 1990)
k_2 = 0.98 d^{-1}, 1.46 d^{-1} \text{ (American flagfish: bioconcentration exptl., toxicity data, Smith et al. 1990)} \\
k_1 = 760 \text{ L kg}^{-1} d^{-1}; \ k_2 = 4.80 d^{-1} \text{ (guppy, 96-h exposure, Sijm et al. 1993)} \\
k_1 = 600 \text{ L kg}^{-1} d^{-1}; \ k_2 = 2.50 d^{-1} \text{ (fathead minnow, 96-h exposure, Sijm et al. 1993)}

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981) \\
t_{1/2} = 200.6–2006 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface Water:

t_{1/2} = 1.1–26 d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980); \\
half-lives from marine mesocosm: t_{1/2} = 18 d in the spring at 8–16°C, t_{1/2} = 10 d in the summer at 20–22°C and t_{1/2} = 31 d in the winter at 3–7°C when volatilization dominates, and t_{1/2} = 10.6 d and 11 d for experiments with and without HgCl_2, respectively, in September 9–15 (Wakeham et al. 1983); \\
hydrolysis t_{1/2} > 900 yr at pH 7 and 25°C (Ellington et al. 1988) \\
t_{1/2}(aerobic) = 672–4320 h, based on unacclimated aerobic screening test data and aerobic soil grab sample data; t_{1/2}(anaerobic) = 2688–17280 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) \\
photolysis t_{1/2} = 25 d under sunlight in water (Mansour & Feicht 1994).

Groundwater: t_{1/2} ~1 yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981) \\
t_{1/2} = 1344–8640 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: t_{1/2} = 672–4320 h, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: t_{1/2} < 1 d in fish tissues (Veith et al. 1980); \\
t_{1/2} < 1 d in bluegill sunfish (Barrows et al. 1980); \\
t_{1/2} = 16 h, clearance from fish (Neely 1980); \\
t_{1/2} < 5 d in worms at 8°C (Oliver 1987a); \\
biological half-lives, t_{1/2} < 1 d in trout muscle, t_{1/2} < 1 d in sunfish and t_{1/2} < 1 d in guppy for dichlorobenzenes (Niimi 1987); \\
depuration t_{1/2} = 0.70 d for whole fish, t_{1/2} = 0.59 d for fish lipid (American flagfish, Smith et al. 1990).
### TABLE 6.1.1.4.1
Reported aqueous solubilities of 1,4-dichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Method</th>
<th>°C</th>
<th>Solubility (g/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>liquid</td>
</tr>
<tr>
<td>Klemenc &amp; Löw 1930</td>
<td>20</td>
<td>68.1</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>79.1</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>93.3</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>104</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>101</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>122</td>
</tr>
<tr>
<td></td>
<td>55</td>
<td>156</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>163</td>
</tr>
<tr>
<td>Wauchope &amp; Getzen 1972</td>
<td>20</td>
<td>22.2</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>24.6</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>25.5</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>30.0</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>38.4</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>47.5</td>
</tr>
<tr>
<td></td>
<td>55</td>
<td>50.1</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>59.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>65.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>65.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>73.4</td>
</tr>
<tr>
<td>Horvath &amp; Getzen 1985 recommended values</td>
<td>10</td>
<td>51.2</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>60.5</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>71.0</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>82.9</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>104.5</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>130</td>
</tr>
<tr>
<td>Shiu et al. 1997 shake flask-GC</td>
<td>5</td>
<td>48.6</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>63.0</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>81.4</td>
</tr>
<tr>
<td></td>
<td>35</td>
<td>104.5</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>130</td>
</tr>
</tbody>
</table>

**FIGURE 6.1.1.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,4-dichlorobenzene.
TABLE 6.1.1.4.2
Reported vapor pressures of 1,4-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

\[
\ln \left( \frac{P}{P_0} \right) = (1 - T/T_o) \cdot \exp \left[ \sum A_i T_i \right] \quad (5) - \text{Cox eq.}
\]

1.

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>McDonald et al. 1959</th>
<th>Walsh &amp; Smith 1961</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>summary of lit. data</td>
<td>ebulliometry</td>
<td>ebulliometry</td>
</tr>
<tr>
<td></td>
<td></td>
<td>manometry</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>54.8</td>
<td>1333</td>
<td>92.0</td>
<td>7605</td>
</tr>
<tr>
<td>69.2</td>
<td>2666</td>
<td>99.41</td>
<td>10114</td>
</tr>
<tr>
<td>84.8</td>
<td>5333</td>
<td>112.6</td>
<td>15600</td>
</tr>
<tr>
<td>95.2</td>
<td>7999</td>
<td>141.65</td>
<td>42066</td>
</tr>
<tr>
<td>108.4</td>
<td>13332</td>
<td>158.52</td>
<td>67660</td>
</tr>
<tr>
<td>128.3</td>
<td>26664</td>
<td>174.12</td>
<td>101325</td>
</tr>
<tr>
<td>150.2</td>
<td>53329</td>
<td>171.87</td>
<td>95945</td>
</tr>
<tr>
<td>173.9</td>
<td>101325</td>
<td>174.04</td>
<td>101325</td>
</tr>
<tr>
<td>mp/°C</td>
<td>53.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\alpha-p\text{-dichlorobenzene}
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>manometry</td>
<td>static manometry</td>
<td>gas saturation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gas saturation-GC</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>37.9</td>
<td>402.6</td>
<td>1.47</td>
<td>14.14</td>
</tr>
<tr>
<td>39.8</td>
<td>469.3</td>
<td>3.94</td>
<td>18.32</td>
</tr>
<tr>
<td>40.2</td>
<td>477.3</td>
<td>6.45</td>
<td>23.67</td>
</tr>
<tr>
<td>40.5</td>
<td>490.6</td>
<td>8.43</td>
<td>28.88</td>
</tr>
<tr>
<td>40.8</td>
<td>501.3</td>
<td>10.33</td>
<td>34.83</td>
</tr>
<tr>
<td>41.1</td>
<td>508.0</td>
<td>12.35</td>
<td>42.44</td>
</tr>
<tr>
<td>41.3</td>
<td>522.6</td>
<td>14.3</td>
<td>51.13</td>
</tr>
<tr>
<td>41.7</td>
<td>534.6</td>
<td>16.63</td>
<td>63.79</td>
</tr>
<tr>
<td>42.4</td>
<td>568.0</td>
<td>19.84</td>
<td>85.98 *solid</td>
</tr>
<tr>
<td>42.6</td>
<td>584.0</td>
<td>16.63</td>
<td></td>
</tr>
<tr>
<td>42.9</td>
<td>593.3</td>
<td>16.63</td>
<td></td>
</tr>
<tr>
<td>43.2</td>
<td>597.3</td>
<td>16.63</td>
<td></td>
</tr>
</tbody>
</table>

\[
\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 64.79
\]

\[
\beta-p\text{-dichlorobenzene}
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>manometry</td>
<td>static manometry</td>
<td>gas saturation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gas saturation-GC</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>37.9</td>
<td>402.6</td>
<td>1.47</td>
<td>14.14</td>
</tr>
<tr>
<td>39.8</td>
<td>469.3</td>
<td>3.94</td>
<td>18.32</td>
</tr>
<tr>
<td>40.2</td>
<td>477.3</td>
<td>6.45</td>
<td>23.67</td>
</tr>
<tr>
<td>40.5</td>
<td>490.6</td>
<td>8.43</td>
<td>28.88</td>
</tr>
<tr>
<td>40.8</td>
<td>501.3</td>
<td>10.33</td>
<td>34.83</td>
</tr>
<tr>
<td>41.1</td>
<td>508.0</td>
<td>12.35</td>
<td>42.44</td>
</tr>
<tr>
<td>41.3</td>
<td>522.6</td>
<td>14.3</td>
<td>51.13</td>
</tr>
<tr>
<td>41.7</td>
<td>534.6</td>
<td>16.63</td>
<td>63.79</td>
</tr>
<tr>
<td>42.4</td>
<td>568.0</td>
<td>19.84</td>
<td>85.98 *solid</td>
</tr>
<tr>
<td>42.6</td>
<td>584.0</td>
<td>16.63</td>
<td></td>
</tr>
<tr>
<td>42.9</td>
<td>593.3</td>
<td>16.63</td>
<td></td>
</tr>
<tr>
<td>43.2</td>
<td>597.3</td>
<td>16.63</td>
<td></td>
</tr>
</tbody>
</table>

\[
\Delta H_{\text{v}}/(kJ \text{ mol}^{-1}) = 35.0
\]
TABLE 6.1.1.4.2 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>manometry</td>
<td>static manometry</td>
<td>gas saturation</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>( t )°C</td>
<td>( \text{P/Pa} )</td>
<td>( t )°C</td>
<td>( \text{P/Pa} )</td>
</tr>
<tr>
<td>43.7</td>
<td>629.3</td>
<td>A</td>
<td>13.6459</td>
</tr>
<tr>
<td>44.1</td>
<td>640.0</td>
<td>B</td>
<td>3431.3</td>
</tr>
<tr>
<td>45.8</td>
<td>727.9</td>
<td>( \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 65.7 )</td>
<td></td>
</tr>
<tr>
<td>46.4</td>
<td>766.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>48.0</td>
<td>859.3</td>
<td>( \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 65.40 )</td>
<td></td>
</tr>
<tr>
<td>49.4</td>
<td>955.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>51.3</td>
<td>955.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>51.7</td>
<td>1135</td>
<td></td>
<td></td>
</tr>
<tr>
<td>52.5</td>
<td>1192</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1</td>
<td>( \text{P/mmHg} )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3.

<table>
<thead>
<tr>
<th>Polednicek et al. 1996</th>
<th>Roháč et al. 1998</th>
<th>Roháč et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>pressure gauge</td>
<td>comparative ebulliometry</td>
<td>recommended</td>
</tr>
<tr>
<td>( t )°C</td>
<td>( \text{P/Pa} )</td>
<td>( t )°C</td>
</tr>
<tr>
<td>solid</td>
<td>liquid</td>
<td></td>
</tr>
<tr>
<td>0.34</td>
<td>12.2</td>
<td>60.12</td>
</tr>
<tr>
<td>0.35</td>
<td>11.98</td>
<td>60.15</td>
</tr>
<tr>
<td>10.35</td>
<td>34.25</td>
<td>70.03</td>
</tr>
<tr>
<td>10.35</td>
<td>34.21</td>
<td>80.03</td>
</tr>
<tr>
<td>20.35</td>
<td>88.75</td>
<td>80.04</td>
</tr>
<tr>
<td>20.35</td>
<td>88.61</td>
<td>89.99</td>
</tr>
<tr>
<td>30.31</td>
<td>214.6</td>
<td>90.0</td>
</tr>
<tr>
<td>40.25</td>
<td>485.5</td>
<td>98.72</td>
</tr>
<tr>
<td>50.15</td>
<td>1037</td>
<td>108.68</td>
</tr>
<tr>
<td>25</td>
<td>135.0</td>
<td>118.73</td>
</tr>
<tr>
<td>interpolated</td>
<td>128.78</td>
<td>28351</td>
</tr>
<tr>
<td>for solid:</td>
<td>138.8</td>
<td>38541</td>
</tr>
<tr>
<td>eq. 3a</td>
<td>148.28</td>
<td>51728</td>
</tr>
<tr>
<td>A</td>
<td>28.4986</td>
<td>68186</td>
</tr>
<tr>
<td>B</td>
<td>6272.86</td>
<td>88642</td>
</tr>
<tr>
<td>C</td>
<td>-32.2741</td>
<td></td>
</tr>
<tr>
<td>for liquid:</td>
<td>172.86</td>
<td>98793</td>
</tr>
<tr>
<td>eq. 3a</td>
<td>175.626</td>
<td>105783</td>
</tr>
<tr>
<td>A</td>
<td>21.0472</td>
<td>173.864</td>
</tr>
<tr>
<td>B</td>
<td>3665.96</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-62.3849</td>
<td></td>
</tr>
<tr>
<td>( \text{P/mmHg} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{P/kPa} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>6.13050</td>
<td>173.864</td>
</tr>
<tr>
<td>B</td>
<td>1575.69</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-65.007</td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
### TABLE 6.1.1.4.2 (Continued)

<table>
<thead>
<tr>
<th>Polednicek et al. 1996</th>
<th>Roháč et al. 1998</th>
<th>Roháč et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>pressure gauge</strong></td>
<td><strong>comparative ebulliometry</strong></td>
<td><strong>recommended</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( P/P_a )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( P/P_a )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( P/P_a )</td>
<td></td>
</tr>
</tbody>
</table>

- \( t/°C \) = 10
- \( P/P_a \) = 3.100023
- \( 10^{-1} A_1 \) = 1.0557743
- \( 10^{-2} A_2 \) = 7.8161354
- \( T_e/K \) = 326.3
- \( P/P_a \) = 1280.0
- \( bp/K \) = 447.01
- temp range 328–449 K

### FIGURE 6.1.1.4.2

Logarithm of vapor pressure versus reciprocal temperature for 1,4-dichlorobenzene.

### TABLE 6.1.1.4.3

Reported Henry’s law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,4-dichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>( \log K_{ow} )</th>
<th>( \log K_{oa} )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ashworth et al. 1988</strong></td>
<td><strong>Bahadur et al. 1997</strong></td>
<td><strong>Su et al. 2002</strong></td>
</tr>
<tr>
<td>( \text{EPICS-GC} )</td>
<td>( \text{shake flask-GC/ECD} )</td>
<td>( \text{GC-RT correlation} )</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( H/(P_a \text{m}^3/\text{mol}) )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( H/(P_a \text{m}^3/\text{mol}) )</td>
<td></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( H/(P_a \text{m}^3/\text{mol}) )</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>215</td>
<td>5</td>
</tr>
<tr>
<td>15</td>
<td>220</td>
<td>15</td>
</tr>
<tr>
<td>20</td>
<td>262</td>
<td>25</td>
</tr>
<tr>
<td>20</td>
<td>321</td>
<td>35</td>
</tr>
<tr>
<td>30</td>
<td>394</td>
<td>45</td>
</tr>
</tbody>
</table>
### TABLE 6.1.1.4.3 (Continued)

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log $K_{OW}$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>EPICS-GC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>$H/(\text{Pa m}^3/\text{mol})$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>Ashworth et al. 1988</td>
<td>$\ln H = A - B/(T/K)$</td>
<td>$A$</td>
</tr>
<tr>
<td>Bahadur et al. 1997</td>
<td>$B$</td>
<td>2720</td>
</tr>
<tr>
<td>Su et al. 2002</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### FIGURE 6.1.1.4.3

Logarithm of Henry's law constant, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,4-dichlorobenzene.
6.1.1.5 1,2,3-Trichlorobenzene

Common Name: 1,2,3-Trichlorobenzene
Synonym: vic-trichlorobenzene
Chemical Name: 1,2,3-trichlorobenzene
CAS Registry No: 81-61-6
Molecular Formula: C₆H₃Cl₃
Molecular Weight: 181.447
Melting Point (°C):
- 51.3 (Lide 2003)
Boiling Point (°C):
- 218.5 (Lide 2003)
Density (g/cm³ at 20°C):
- 1.4533 (40°C, Weast 1972–73; Horvath 1982)
- 1.4533 (25°C, Lide 2003)
- 1.69 (Dean 1985, 1992)
Molar Volume (cm³/mol):
- 124.9 (25°C, calculated-density)
- 158.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
- 17.364 (Tsonopoulos & Prausnitz 1971)
- 17.99 (Miller et al. 1984)
- 17.153 (Ruelle et al. 1993)
- 20.50 (Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
- 53.14 (Tsonopoulos & Prausnitz 1971)
- 56.90 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
- 0.552 (mp at 51.3°C)
- 0.53 (25°C, mp at 53°C, Suntio et al. 1988b)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 25.1 (Tsonopoulos & Prausnitz 1971)
- 31.5 (shake flask-UV, Yalkowsky et al. 1979, 1983)
- 16.6 (shake flask-GC, Mackay & Shiu 1981)
- 12.0 (shake flask-GC, Könemann 1981)
- 31.6 (recommended, Horvath 1982)
- 12.27 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 18.0 (shake flask-HPLC, Banerjee 1984)
- 16.3 (23°C, shake flask-GC, Chiou 1985)
- 18.0 (shake flask-GC, Chiou et al. 1986; Chiou et al. 1991)
- 19.5* ± 0.24; 23.7 ± 1.3 (generator column-GC/ECD; shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
- 13.0 (shake flask-GC, Boyd et al. 1998)
\[ \ln x = -1.773 - 3418.9/(T/K), \text{ temp range } 5–50\degree C \text{ (regression eq. of literature data, Shiu & Ma 2000)} \]
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 133.3* (40°C, summary of literature data, Stull 1947)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics 1299

52.4 (extrapolated-Antoine eq., supercooled liquid P_L, Weast 1972–73)
log (P/mmHg) = [-0.2185 × 11349.5/(T/K)] + 7.91649; temp range 40–218.5°C (Antoine eq., Weast 1972–73)
28.0 (selected-converted from reported P_L, with fugacity ratio, Mackay & Shiu 1981)
25.1 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
17.7 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.23008 – 2624.09/(10.506 + T/K); temp range 343–492 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

8.82* (20.35°C, static method-pressure gauge measurement; Antoine eq., measured range 0.36–169°C, Polednicek et al. 1996)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
127 (gas stripping-GC, Mackay & Shiu 1981)
90.0 (gas stripping-GC, Oliver 1985)
72.0 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
147 (equilibrium air stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log KOW at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.27 (Leo et al. 1971; Hansch & Leo 1979)
4.11, 3.99 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)
4.02 (HPLC-k’ correlation, McDuffie 1981)
3.97 (shake flask-GC, Watarai et al. 1982)
3.96 (HPLC-k’ correlation, Hammers et al. 1982)
4.04 (generator column-GC, Miller et al. 1984, 1985)
4.14 (shake flask-GC, Chiou 1985)
4.14 (shake flask-GC, Pereira et al. 1988)
4.139 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
4.05 (recommended, Sangster 1993)
4.14* (recommended, Hansch et al. 1995)
3.81* (estimated- RP-HPLC-k’ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log KOA at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
5.19*, 5.11 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
log K_OA = –4.6 + 20–8.7/(T/K); ΔH_OA = 55.7 kJ/mol (Harner & Mackay 1995)
5.19 (calculated-S_ect and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
4.11 (guppy, lipid basis, Könemann & van Leeuwen 1980)
3.00–3.20 mean 3.08; 3.34–3.52 mean 3.41 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.15–4.47 (rainbow trout, lipid basis, Oliver & Niimi 1983)
3.08–3.42 (fish, Oliver 1984)
4.35 (rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
4.11 (guppy, 5.4% lipid, wet wt basis, Geyer et al. 1985)
4.11 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1987, 1989)
2.85 (fish, calculated-concentration ratio C_d/C_w or rate constant ratio k_1/k_2, Connell & Hawker 1988)
3.28 (guppy, Van Hoogen & Opperhuizen 1988)
4.76, 4.90, 3.54, 4.68 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.30 (guppy, steady-state conditions, rate const. ratio k_1/k_2, 96-h exposure, Sijm et al. 1993)
4.50 (guppy, lipid normalized BCF, Sijm et al. 1993)
2.99 (Scenedesmus spp. Coenobia, dry wt., batch adsorption, Koelmans et al. 1993)
2.90, 3.28; 3.08, 3.41 (Poecilia reticulata; Oncorhynchus mykiss, quoted lit., flow through conditions, Devillers et al. 1996)
2.94–3.23 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
3.08, 4.16; 2.812, 3.055 (quoted: whole fish, lipid content; calculated- MCI χ, K_mow, Lu et al. 1999)
3.68; 3.72 (Oncorhynchus mykiss, wet wt. basis: quoted exppt.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_OC:
2.85 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
2.73–4.00 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
4.70; 4.10 (field data of Lake Ontario sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
3.0, 2.0 (Sanhedron soil humic acid, Suwanee River humic acid, batch equilibrium-sorption isotherm, GC/ECD, Chioi et al. 1986)
2.3, 2.0 (Sanhedron soil fulvic acid, Suwanee River fulvic acid, batch equilibrium-sorption isotherm, GC/ECD, Chioi et al. 1986)
3.21, 3.14 (Riddles soil: top layer 1.84% OC; below top layer, batch equilibrium-sorption isotherm, Boyd et al. 1990)
3.18, 3.38, 3.43, 3.26, 3.23 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
3.91 (Isora soil 1.87% OC, batch equilibrium, GC, Paya-Perez et al. 1991)
3.81 (lake sediment 2.5% OC, batch equilibrium, Schrap et al. 1994)
3.61 ± 0.39 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.16 (HPLC-screening method; Müller & Kördel 2001)
3.48, 3.37 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environment Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH} ~ 1.0 × 10^{-13} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}, \text{residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981) }
\text{k(aq.)} \leq 0.06 \text{M}^{-1} \text{s}^{-1} \text{for direct reaction with ozone in water at pH 3 and 21°C, with t}_5 > 6 \text{d at pH 7 (Yao & Haag 1991). }
k_{NO_3,calc} = 4.0 \times 10^9 \text{M}^{-1} \text{s}^{-1} \text{in aqueous solutions (Haag & Yao 1992) }
Hydrolysis: base rate constant k < 0.9 M^{-1} h^{-1} at 25°C with a calculated t_5 > 900 yr at pH 7 (Ellington et al. 1988)
Biodegradation: dechlorination pseudo-first order rate constant k = 0.387 d^{-1} with t_5 = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
k_1 = 8300 \text{d}^{-1}; k_2 = 0.45 \text{d}^{-1} (guppy, exppt., Könemann & van Leeuwen 1980)
k_2 = 0.45 \text{d}^{-1} (guppy, exppt., Könemann & van Leeuwen 1980)
Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water: $t_{1/2} = 1.9–30$ d, surface waters in various locations in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

Hydrolysis $t_{1/2} > 900$ yr at pH 7 and 25°C (Ellington et al. 1988)

$k(\text{exptl}) \leq 0.006$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} > 6$ d at pH 7 (Yao & Haag 1991)

Groundwater:

Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological $t_{1/2} < 1$ d in trout, $t_{1/2} = 2$ d in sunfish and $t_{1/2} = 2$ d in guppy for trichlorobenzenes (Niimi 1987)

$\tau_{1/2} < 5$ d in worm at 8°C (Oliver 1987a).

### TABLE 6.1.1.5.1

Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3-trichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>log $K_{OW}$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shiu et al. 1997</td>
<td>log $K_{OW}$</td>
<td>log $K_{OA}$</td>
</tr>
<tr>
<td>shake flask-GC</td>
<td>generator column-GC/ECD</td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S$/g·m$^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>7.66</td>
<td>5</td>
</tr>
<tr>
<td>25</td>
<td>19.31</td>
<td>15</td>
</tr>
<tr>
<td>50</td>
<td>45.61</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>35</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\Delta H_{OA}/(kJ$ mol$^{-1}) = 55.7$

$log K_{OA} = A + B/T$

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.6</td>
<td>2909</td>
</tr>
</tbody>
</table>
**FIGURE 6.1.1.5.1** Logarithm of mole fraction solubility, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,2,3-trichlorobenzene.
TABLE 6.1.1.5.2
Reported vapor pressures of 1,2,3-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \quad \ln P = A - \frac{B}{T/K} \quad (1a)
\]
\[
\log P = A - \frac{B}{C + t/°C} \quad (2) \quad \ln P = A - \frac{B}{C + t/°C} \quad (2a)
\]
\[
\log P = A - \frac{B}{C + T/K} \quad (3) \quad \ln P = A - \frac{B}{C + T/K} \quad (3a)
\]
\[
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]
\[
\ln \left( \frac{P}{P_0} \right) = (1 - T/T_o) \cdot \exp \left[ \sum A_i T_i \right] \quad \text{- Cox eq.} \quad (5)
\]

1. 

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>( P/Pa )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>40</td>
<td>133.3</td>
<td>0.36</td>
</tr>
<tr>
<td>70</td>
<td>666.6</td>
<td>0.38</td>
</tr>
<tr>
<td>85.5</td>
<td>1333</td>
<td>10.35</td>
</tr>
<tr>
<td>101.8</td>
<td>2666</td>
<td>10.36</td>
</tr>
<tr>
<td>119.8</td>
<td>5333</td>
<td>20.35</td>
</tr>
<tr>
<td>131.5</td>
<td>7999</td>
<td>20.37</td>
</tr>
<tr>
<td>146.0</td>
<td>13332</td>
<td>30.28</td>
</tr>
<tr>
<td>168.2</td>
<td>26664</td>
<td>30.28</td>
</tr>
<tr>
<td>193.5</td>
<td>53329</td>
<td>50.12</td>
</tr>
<tr>
<td>218.5</td>
<td>101325</td>
<td>50.12</td>
</tr>
<tr>
<td>( \Delta H_{\text{subl}}/(kJ \ mol^{-1}) = 72.7 )</td>
<td>25</td>
<td>14.07</td>
</tr>
<tr>
<td>( mp/°C )</td>
<td>52.5</td>
<td>interpolated</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 3a</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2. 

Roháč et al. 1999

<table>
<thead>
<tr>
<th>Summary of Lit. Data</th>
<th>Polednicek et al. 1996</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T/K )</td>
<td>( P/Pa )</td>
</tr>
<tr>
<td>solid</td>
<td>liquid</td>
</tr>
<tr>
<td>233.15</td>
<td>0.003</td>
</tr>
<tr>
<td>243.15</td>
<td>0.015</td>
</tr>
<tr>
<td>253.15</td>
<td>0.065</td>
</tr>
</tbody>
</table>

(Continued)
**TABLE 6.1.1.5.2 (Continued)**

Roháč et al. 1999

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>263.15</td>
<td>0.26</td>
<td>363.15</td>
<td>1329</td>
</tr>
<tr>
<td>273.15</td>
<td>0.90</td>
<td>373.15</td>
<td>2106</td>
</tr>
<tr>
<td>283.15</td>
<td>2.90</td>
<td>383.15</td>
<td>3245</td>
</tr>
<tr>
<td>283.15</td>
<td>8.50</td>
<td>393.15</td>
<td>4868</td>
</tr>
<tr>
<td>303.15</td>
<td>23.1</td>
<td>403.15</td>
<td>7130</td>
</tr>
<tr>
<td>313.15</td>
<td>58.9</td>
<td>413.15</td>
<td>10220</td>
</tr>
<tr>
<td>323.15</td>
<td>140.9</td>
<td>423.15</td>
<td>14340</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Data fitted to Cox eq. 443.15 26760
For solid eq. 5 P/Pa 463.15 46860
A0 3.380608 10–4A1 –2.5802866 A2 0
T/K 325.6 494.45 Cox eq.
bp/K 173.0 494.45
temp range 273–323 K

**FIGURE 6.1.1.5.2** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trichlorobenzene.
6.1.1.6 1,2,4-Trichlorobenzene

![Structure of 1,2,4-Trichlorobenzene](image)

Common Name: 1,2,4-Trichlorobenzene
Synonym: unsym-trichlorobenzene
Chemical Name: 1,2,4-trichlorobenzene
CAS Registry No: 120-82-1
Molecular Formula: C₆H₃Cl₃
Molecular Weight: 181.447
Melting Point (°C):
16.92 (Lide 2003)
Boiling Point (°C):
213.5 (Weast 1972–73; Lide 2003)
Density (g/cm³ at 20°C):
1.4542 (Weast 1972–73)
1.446 (Dean 1985, 1992)
1.459 (Lide 2003)
Molar Volume (cm³/mol):
124.8 (20°C, calculated-density)
158.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.48 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.56 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio, at 25°C, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25.03 (Irmann 1965)
34.7 (shake flask-UV, Yalkowsky et al. 1979)
30.0 (Callahan et al. 1979)
19.4 (shake flask-GC, Könenmann 1981)
30.0 (recommended, Hovarth 1982)
48.8 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; 1983)
46.1 (generator column-GC/ECD, Miller et al. 1984; 1985)
31.3 (shake flask-HPLC/UV, Banerjee 1984)
30.9 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
34.6 (shake flask-GC, Chiou 1985)
52.0 (shake flask-GC, Boyd et al. 1998)
36.5* ± 0.36 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (38.4°C, summary of literature data, temp range 38.4–213°C, Stull 1947)
38.6 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.19608 – 1827.0/(210.0 + t°C); temp range 110–280°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [–0.2185 × 11425.1/(T/K)] + 8.030523; temp range 38.4–213°C (Antoine eq., Weast 1972–73)
Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals

26.4 (gas saturation, Politzki et al. 1982)
28.5 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
38.7 (interpolated-Antoine eq-III, Stephenson & Malanowski 1987)

\[
\log (P_{v}/kPa) = 9.570 - 3254/(T/K); \text{ temp range 279–290 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P_{v}/kPa) = 6.31998 - 1827/(−63.15 + T/K); \text{ temp range 383–553 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P_{v}/kPa) = 6.6802 - 2064.4/(−43.05 + T/K); \text{ temp range 293–383 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)}
\]

53.4 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)

\[
\log (P_{v}/kPa) = 9.570 - 3254/(T/K); \text{ temp range 6–17°C (solid, regression eq. from literature data, Shiu & Ma 2000)}
\]

\[
\log (P_{v}/kPa) = 6.682 - 2064.4/(−43.05 + T/K); \text{ temp range 20–110°C (liquid, regression eq. from literature data, Shiu & Ma 2000)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

122 (gas stripping-GC, Oliver 1985)
144 (gas stripping-GC, Warner et al. 1987)
195* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

\[
\ln [H/(atm·m^3/mol)] = −16.34 + 3307/(T/K); \text{ temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)}
\]

101 (gas stripping-GC, ten Hulscher et al. 1992)
375.2 (modified EPICS method-GC, Ryu & Park 1999)

172 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

\[
\log K_{AW} = 4.381 - 1622/(T/K) \text{ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.05 (Leo et al. 1971)
4.26 (Callahan et al. 1979)
4.02 (Hansch & Leo 1979; Hansch & Leo 1985)
3.93 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)
4.02 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; Chiou 1985)
3.97 (shake flask-GC, Watarai et al. 1982)
3.96 (HPLC-k’ correlation, Hammers et al. 1982)

3.93–4.18, 4.09 (range, mean, shake flask method, Eadsforth & Moser 1983)
4.12–4.32, 4.21 (range, mean, HPLC method, Eadsforth & Moser 1983)
3.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
4.22 (HPLC-k’ correlation, De Kock & Lord 1987)
4.02 (shake flask-GC, Pereira et al. 1988)
4.05 (slow stirring-GC, De Bruijn et al. 1989)
4.02 (recommended, Sangster 1993)
4.02 (recommended, Hansch et al. 1995)
3.92* (estimated- RP-HPLC-k’ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.

5.10* (20°C, HPLC-k’ correlation, measured range 10–50°C, Su et al. 2002)

\[
\log K_{OA} = 62080/(2.303·RT) – 6.031; \text{ temp range 10–50°C (HPLC-k’ correlation, Su et al. 2002)}
\]
### Bioconcentration Factor, log BCF at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Species/Condition</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.32</td>
<td>fathead minnow, 32-d exposure</td>
<td>Veith et al. 1979b</td>
</tr>
<tr>
<td>3.45; 3.37; 2.95</td>
<td>fathead minnow; green sunfish; rainbow trout</td>
<td>Veith et al. 1979b</td>
</tr>
<tr>
<td>2.69</td>
<td>fish, flowing water</td>
<td>Kenaga &amp; Goring 1980; Kenaga 1980a</td>
</tr>
<tr>
<td>2.26</td>
<td>bluegill sunfish, whole body, flow system</td>
<td>Barrows et al. 1980</td>
</tr>
<tr>
<td>3.52</td>
<td>microorganism-water</td>
<td>Mabey et al. 1982</td>
</tr>
<tr>
<td>3.04–3.11</td>
<td>mean 3.11</td>
<td>(rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver &amp; Niimi 1983)</td>
</tr>
<tr>
<td>4.19–4.56</td>
<td>(rainbow trout, lipid base, Oliver &amp; Niimi 1983)</td>
<td></td>
</tr>
<tr>
<td>3.26–3.61</td>
<td>(fish, Oliver 1984, 1985)</td>
<td></td>
</tr>
<tr>
<td>2.40</td>
<td>(algae, Oliver et al. 1984)</td>
<td></td>
</tr>
<tr>
<td>2.40, 2.69, 3.15</td>
<td>(algae, fish, sludge, Klein et al. 1984)</td>
<td></td>
</tr>
<tr>
<td>3.15–3.72</td>
<td>mean 3.36; 3.30–3.75 mean 3.57 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver &amp; Niimi 1985)</td>
<td></td>
</tr>
<tr>
<td>3.11; 3.08</td>
<td>(rainbow trout, wet wt. basis, laboratory data; Lake Ontario field data, Oliver &amp; Niimi 1985)</td>
<td></td>
</tr>
<tr>
<td>4.19–4.56</td>
<td>(rainbow trout, lipid base, Oliver &amp; Niimi 1985)</td>
<td></td>
</tr>
<tr>
<td>2.09; 3.84</td>
<td>(quoted, rainbow trout, 1.8% lipid, wet wt basis, lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.28, 2.40, 2.34, 2.66</td>
<td>(quoted, carp, 2.2% lipid, wet wt basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>3.94, 3.96, 4.0, 4.32</td>
<td>(quoted, carp, 2.2% lipid, lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.54; 4.04</td>
<td>(quoted, rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Oliver &amp; Niimi 1985)</td>
<td></td>
</tr>
<tr>
<td>2.66, 2.73; 4.02, 4.09</td>
<td>(quoted, carp, 4.4% lipid, wet wt basis, lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.96; 4.26</td>
<td>(quoted, golden ide, 5.0% lipid, wet wt basis, lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.86, 2.94; 4.15, 4.19</td>
<td>(quoted, zebra fish, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.83, 3.12; 4.12, 4.22</td>
<td>(quoted, tilapia, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.98, 3.12; 4.23, 4.36</td>
<td>(quoted, bluegill sunfish, 5.7% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>3.13, 3.14; 4.37, 4.38</td>
<td>(quoted, guppy, 5.8% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>3.11, 3.20; 4.23, 4.38</td>
<td>(quoted, rainbow trout, 7.7%, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.96, 3.03; 4.05, 4.23</td>
<td>(quoted, guppy, 8.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>3.11; 4.19</td>
<td>(quoted, rainbow trout, 8.3% lipid, wet wt basis; lipid basis, Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>3.32; 4.30</td>
<td>(quoted, fathead minnow, 10.5% lipid, wet wt basis, lipid basis Geyer et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.69; 2.40; 3.15</td>
<td>(fish; algae; activated sludge, Freitag et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>2.61</td>
<td>(fathead minnow, Carlson &amp; Kosian 1987)</td>
<td></td>
</tr>
<tr>
<td>4.76, 4.90, 3.54, 4.68</td>
<td>(field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)</td>
<td></td>
</tr>
<tr>
<td>3.31, 4.25</td>
<td>(American flagfish, whole fish, fish lipid, Smith et al. 1990)</td>
<td></td>
</tr>
<tr>
<td>2.95–3.57; 3.31; 3.32; 3.36</td>
<td>(Oncorhynchus mykiss; Jordanella floridae; Pimephales promelas; Lepomis cyanellus, quoted lit., flow through conditions, Devillers et al. 1996)</td>
<td></td>
</tr>
<tr>
<td>3.0, 3.06, 3.06</td>
<td>(guppy: k&lt;sub&gt;1&lt;/sub&gt;/k&lt;sub&gt;2&lt;/sub&gt;-best fit exptl. data, k&lt;sub&gt;1&lt;/sub&gt;/k&lt;sub&gt;2&lt;/sub&gt;-slope method, C&lt;sub&gt;f&lt;/sub&gt;/C&lt;sub&gt;w&lt;/sub&gt;-steady state, van Eck et al. 1997)</td>
<td></td>
</tr>
<tr>
<td>3.81; 3.89</td>
<td>(Oncorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)</td>
<td></td>
</tr>
</tbody>
</table>

### Sorption Partition Coefficient, log K<sub>OC</sub>:

<table>
<thead>
<tr>
<th>Value</th>
<th>Condition/Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.80</td>
<td>river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach &amp; Westall 1981</td>
</tr>
<tr>
<td>2.68–3.94</td>
<td>(5 soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach &amp; Westall 1981)</td>
</tr>
<tr>
<td>4.70; 4.40</td>
<td>(field data of sediment trap material; Niagara River-organic matter; Oliver &amp; Charlton 1984)</td>
</tr>
<tr>
<td>4.3–5.1, 5.10</td>
<td>(suspended sediment, average; algae &gt; 50 µm, Oliver 1987c)</td>
</tr>
<tr>
<td>4.8–5.3, 5.0</td>
<td>(Niagara River plume, range, mean, Oliver 1987b)</td>
</tr>
<tr>
<td>3.91</td>
<td>(untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)</td>
</tr>
<tr>
<td>3.27</td>
<td>(untreated Marlette soil B, horizon, 0.30% OC, equilibrium isotherm, Lee et al. 1989)</td>
</tr>
</tbody>
</table>
3.91, 3.64, 3.04 (organic cations treated Marlette soil B horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.32 (calculated-K_{OM}, Aldrich or Fluka humic acid polymers, Chin & Weber 1989)
3.32; 2.62 (Aldrich humic acid, organic polymers, Chin et al. 1990)
4.02 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
2.71, 2.71 (RP-HPLC-k' correlation including: MCI-related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
3.86 ± 0.40 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.15, 3.19, 3.10 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
4.38–3.24 (NIST SRM diesel particulate matter, sorption isotherm, Nguyen et al. 2004)

Sorption Partition Coefficient, log K_{OM}: 
2.70 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.97 (untreated Marlette soil B horizon, 0.30% OC, equilibrium sorption isotherm, Lee et al. 1989)
3.97, 3.50, 2.87 (organic cations treated Marlette soil B horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives. t_½: 
Volatileization: rate constants: k = 0.032 d⁻¹ with t_½ = 22 d in spring at 8–16°C, k = 0.066 d⁻¹ with t_½ = 11 d in summer at 20–22°C, k = 0.058 d⁻¹ with t_½ = 12 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.073 d⁻¹ with t_½ = 9.5 d with HgCl₂, and k = 0.066 d⁻¹ with t_½ = 10.6 d without HgCl₂ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)
Photolysis: not environmentally relevant (Mabey et al. 1982)
 k = 1.16 × 10⁻³ h⁻¹ with H₂O₂ at 25°C in F-113 solution and with HO⁻ in the gas (Dilling et al. 1988)
k = 0.03 h⁻¹, the maximum summer photolysis rate calculated at midday clear sky, the minimum photolytic t_½ ~ 4 months, but a realistic value is likely to be at least 1 yr (Bunce et al. 1989)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:
k = 7.22 × 10⁻³ h⁻¹ (Simmons et al. 1976; selected, Mackay et al. 1985)
k_{OH} ~ 1.0 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
k_{(singlet oxygen)} << 360 M⁻¹ h⁻¹; k (RO₂ radical) << 1 M⁻¹ h⁻¹ (Mabey et al. 1982)
k << 1.6 M⁻¹ s⁻¹ for the reaction with ozone in water using 10 mM t-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)
k_{OH} = 5.32 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 296 K, measured range 273–368 K (flash photolysis-resonance fluorescence, Rinke & Zetzsch 1984)
k_{OH} (obs.) = 5.32 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹; and k_{OH}(calc) = 3.47 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)
k_{O₂(calc)} = 0.29 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, k_{O₂(obs)} = 0.532 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH(aq.)} = 4.0 × 10⁶ M⁻¹ s⁻¹ in aqueous solutions (Haag & Yao 1992)
k_{OH(calc)} = 0.34 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)
Hydrolysis: not environmentally significant (Mabey et al. 1982);
base rate constant k < 0.9 M⁻¹ h⁻¹ at 25°C with a calculated t_½ > 900 yr at pH 7 (Ellington et al. 1988)
first-order rate constant k = 2.3 × 10⁻⁵ h⁻¹ with t_½ = 3.4 yr at pH 7 and 25°C (Howard et al. 1991).
Biodegradation: k = 1.92 × 10⁻² h⁻¹, degradation in water (Simmons et al. 1976)
t_{(aq. aerobic)} = 672–4320 h estimated from unacclimated soil grab sample data (Howard et al. 1991)
t_{(aq. anaerobic)} = 2688–17280 h based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

\[ k = 0.05 \text{ d}^{-1}, \text{ significant degradation in an aerobic environment (Tabak et al. 1981; Mills 1982)} \]

\[ k = 0.029 \text{ d}^{-1} \text{ in river water, } k = 0.026 \text{ d}^{-1} \text{ in estuarine water, and } k = 0.012 \text{ d}^{-1} \text{ in marine water (Bartholomew & Pfander 1983; Battersby 1990)} \]

\[ t_{1/2}(\text{aerobic}) = 28 \text{ d}, t_{1/2}(\text{anaerobic}) = 110 \text{ d} \text{ in natural waters (Capel & Larson 1995)} \]

\[ k = 0.035 \text{ d}^{-1}, \text{ the dechlorination pseudo-first order rate constant, with } t_{1/2} = 19.8 \text{ d} \text{ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)} \]

Biotransformation: \( 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1} \) (estimated, Mabey et al. 1982).

Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

\[ k_1 = 8300 \text{ d}^{-1}; k_2 = 0.45 \text{ d}^{-1} \text{ (guppy, exptl., Könenmann & Van Leeuwen 1980)} \]

\[ k_1 = 18.7 \text{ h}^{-1}; 1/k_2 = 53.0 \text{ h} \text{ (guppy, selected, Hawker & Connell 1985)} \]

\[ \log k_1 = 2.65 \text{ d}^{-1}; \log 1/k_2 = 0.34 \text{ d} \text{ (guppy, selected, Connell & Hawker 1988)} \]

\[ \log k_1 = -1.85 \text{ d}^{-1}; \log k_2 = 0.23 \text{ d}^{-1} \text{ (fish, calculated-KOW, fast-biphasic, Thomann 1989)} \]

\[ t_{1/2} = 1158 \text{ d}^{-1}, 10140 \text{ d}^{-1}; k_2 = 0.57 \text{ d}^{-1}, 0.57 \text{ d}^{-1} \text{ (American flagfish: whole fish, fish lipid, Smith et al. 1990)} \]

\[ k_1 = 492 \pm 234 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.49 \pm 0.22 \text{ d}^{-1} \text{ (guppy, exptl., van Eck et al. 1997)} \]

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

- calculated minimum photolytic \( t_{1/2} \approx 4 \text{ months} \), but realistically at least 1 yr (Bunce et al. 1989);
- tropospheric lifetime of 25 d based on reaction principally with OH radical and other photochemical reactions (Bunce 1991);

\[ t_{1/2} = 128.4–1284 \text{ h}, \text{ based on the photooxidation with OH radical (Howard et al. 1991)} \]

Surface Water: \( t_{1/2} = 2.1–28 \text{ d} \text{ estimated for various locations in the Netherlands, } t_{1/2} = 0.3–3 \text{ d} \text{ for river water, } t_{1/2} = 3–30 \text{ d} \text{ for lakes estimated from persistence (Zoeteman et al. 1980)}; \)

- half-lives from marine mesocosm: \( t_{1/2} = 22 \text{ d} \text{ in the spring at } 8–16{\degree}C, t_{1/2} = 11 \text{ d} \text{ in the summer at } 20–22{\degree}C \)
- and \( t_{1/2} = 12 \text{ d} \text{ in the winter at } 3–7{\degree}C \text{ when volatilization dominates, and } t_{1/2} = 9.5 \text{ d} \text{ and } 10.6 \text{ d} \text{ for experiments with and without HgCl}_2, \text{ respectively in September 9–15 (Wakeham et al. 1983)} \)

- hydrolysis \( t_{1/2} > 900 \text{ yr} \text{ at pH 7 and } 25{\degree}C \) (Ellington et al. 1988)

\[ t_{1/2}(\text{aerobic}) = 672–4320 \text{ h}, \text{ based on unacclimated aerobic soil grab sample data; } t_{1/2}(\text{anaerobic}) = 2688–17280 \text{ h, based on estimated unacclimated aerobic biodegradation half-life; and first order hydrolysis \( t_{1/2} = 3.4 \text{ yr} \) (Howard et al. 1991)}; \]

\[ t_{1/2}(\text{aerobic}) = 28 \text{ d}, t_{1/2}(\text{anaerobic}) = 110 \text{ d} \text{ in natural waters (Capel & Larson 1995)} \]

Groundwater: \( t_{1/2} = 1344–8640 \text{ h}, \text{ based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}; \)

\[ t_{1/2} = 30–300 \text{ d} \text{ estimated from persistence (Zoeteman et al. 1980)} \]

Soil: \( t_{1/2} < 10 \text{ d} \) (Ryan et al. 1988)

\[ t_{1/2} = 672–4320 \text{ h}, \text{ based on unacclimated aerobic soil grab sample data (Howard et al. 1991)} \]

Sediment: dechlorination \( t_{1/2} = 19.8 \text{ d} \text{ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)} \)

Biota: \( 1 < t_{1/2} < 3 \text{ d} \text{ in blue bluegill sunfish (Barrows et al. 1980)}; \)

- biological half-lives, \( t_{1/2} < 1 \text{ d} \text{ in trout, } t_{1/2} = 2 \text{ d} \text{ in sunfish, and } t_{1/2} = 2 \text{ d} \text{ in guppy for trichlorobenzenes (Niimi 1987)}; \)

- \( t_{1/2} < 5 \text{ d} \text{ in worms at } 8{\degree}C \) (Oliver 1987a);

- depuration \( t_{1/2} = 1.21 \text{ d} \text{ from whole fish, } t_{1/2} = 1.20 \text{ d} \text{ from fish lipid (American flagfish, Smith et al. 1990)} \).
TABLE 6.1.1.6.1  
Reported aqueous solubilities of 1,2,4-trichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>32.9</td>
<td>5</td>
<td>7.71</td>
</tr>
<tr>
<td>15</td>
<td>28.5</td>
<td>15</td>
<td>10.39</td>
</tr>
<tr>
<td>25</td>
<td>36.5</td>
<td>25</td>
<td>13.58</td>
</tr>
<tr>
<td>35</td>
<td>39.8</td>
<td>35</td>
<td>19.82</td>
</tr>
<tr>
<td>45</td>
<td>46.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.1.6.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2,4-trichlorobenzene.
TABLE 6.1.6.2
Reported vapor pressures of 1,2,4-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[ \log P = A - \frac{B}{T/K} \]  
\[ \ln P = A - \frac{B}{T/K} \]  
\[ \log P = A - \frac{B}{C + T/K} \]  
\[ \ln P = A - \frac{B}{C + T/K} \]  
\[ \ln \left( \frac{P}{P_0} \right) = \left(1 - \frac{T}{T_0}\right) \exp \left[ \sum A_i T^i \right] \] - Cox eq.

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/Pa</th>
<th>Stoll 1947</th>
<th>Sears &amp; Hopke 1949</th>
<th>comparative ebulliometry</th>
<th>Roháč et al. 1998</th>
<th>Roháč et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>measured range: 6–25°C</td>
<td>17.05–17.40</td>
<td>eq. 1 P/micron</td>
<td>for solid:</td>
<td>for liquid:</td>
</tr>
<tr>
<td>38.4</td>
<td>133.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>67.3</td>
<td>666.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>81.7</td>
<td>1333</td>
<td>mp/°C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>97.2</td>
<td>2666</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>114.8</td>
<td>5333</td>
<td>for solid:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>125.7</td>
<td>7999</td>
<td>eq. 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>13332</td>
<td>B</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>162</td>
<td>26664</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>187.7</td>
<td>53329</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>213</td>
<td>101325</td>
<td>for liquid:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>17.0</td>
<td>A</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>213</td>
<td>101325</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>bp/°C</td>
<td>213,492</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 3</td>
<td>P/kPa</td>
<td>eq. 5</td>
<td>P/Pa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>6.11973</td>
<td>( A_1 )</td>
<td>3.352607</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1677.35</td>
<td>( 10^{3}A_1 )</td>
<td>-9.0343639</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-78.926</td>
<td>( 10^{7}A_2 )</td>
<td>6.0501757</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T/K</td>
<td>290.07</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P/Pa</td>
<td>19.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>bp/K</td>
<td>486.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>temp range</td>
<td>294–489 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 6.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.3
Reported Henry’s law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4-trichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log $K_{OW}$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ashworth et al. 1988</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPICS-GC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$H/(Pa m^3/mol)$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>10</td>
<td>131</td>
<td>5</td>
</tr>
<tr>
<td>15</td>
<td>106</td>
<td>15</td>
</tr>
<tr>
<td>20</td>
<td>185</td>
<td>25</td>
</tr>
<tr>
<td>30</td>
<td>301</td>
<td>35</td>
</tr>
</tbody>
</table>

$\ln (H/(atm m^3/mol)) = A - B/(T/K)$

| A | 7.261 |
| B | 4028  |

$\Delta H_OA/(kJ mol^{-1}) = 62.08$

$\log K_{OA} = A + B/2.303RT$

| A | -6.031 |
| B | 62080  |
FIGURE 6.1.1.6.3 Logarithm of Henry's law constant, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,2,4-trichlorobenzene.
6.1.1.7 1,3,5-Trichlorobenzene

Common Name: 1,3,5-Trichlorobenzene
Synonym: sym-trichlorobenzene
Chemical Name: 1,3,5-trichlorobenzene
CAS Registry No: 108-70-3
Molecular Formula: C₆H₃Cl₃
Molecular Weight: 181.447

Melting Point (°C):
62.8 (Lide 2003)

Boiling Point (°C):
208.0 (Weast 1972–72, 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
1.3865 (64°C, Weast 1972–73; Horvath 1982)

Molar Volume (cm³/mol):
130.9 (64°C, calculated-density)
125 (calculated-density, liquid molar volume, Chiou 1985)
158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
19.622 (Tsonopoulos & Prausnitz 1971)
18.786 (Miller et al. 1984)
18.198 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ∆Sₐ₃ (J/mol K):
58.16 (Tsonopoulos & Prausnitz 1971)
56.07 (Miller et al. 1984)

Fugacity Ratio at 25°C (assuming ∆Sₐ₃ = 56 J/mol K), F: 0.426 (mp at 62.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25.03 (Tsonopoulos & Prausnitz 1971)
6.59 (shake flask-UV, Yalkowsky et al. 1979)
5.87 (shake flask-GC, Könemann 1981)
6.61 (recommended, Hovarth 1982)
4.12 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.01 (shake flask-HPLC, Banerjee 1984)
10.6 (shake flask-GC, Chiou 1985)
6.53 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
8.46* ± 0.26 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
2.40 (shake flask-GC, Boyd et al. 1998)
ln x = –5.083768 – 2650.68/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
666.6* (63.8°C, summary of literature data, temp range 63.8–208.4°C, Stull 1947)
77 (extrapolated Antoine eq., supercooled liquid, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 11211.0/(T/K)] + 7.977218; temp range 63.8–208.4°C (Antoine eq., Weast 1972–73)
30.23 (gas saturation, interpolated from reported graph, Rordorf 1985)
24.4 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 8.301 – 2956/(T/K); temp range 282–301 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 6.43345 – 1932.26/(-45.268 + T/K); temp range 336–482 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

124.4 (GC-RT correlation, Watanabe & Tatsukawa 1989)

62.4; 74.9 (supercooled liquid P_L, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)

log (P_L/mmHg) = 19.2854 – 4.4976 × 10^-3 × (T/K) – 3.6158 × 10^-5 × (T/K)^2, temp range 398–748 K (Yaws 1994)

12.4, 20.44* (20.35°C pressure gauge measurement, 25°C interpolated from reported Antoine eq. based on exptl. data, Polednicek et al. 1996)

ln (P_s/Pa) = 32.5109 – 8909.70/[T(K) + 3.94116]; temp range 273–333 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)

ln (P_L/Pa) = 21.1215 – 3939.96/[T(K) – 71.2907]; temp range 343–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)

Henry’s Law Constant (Pa m^3/mol at 25°C):

192.5 (20°C, batch stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

4.02 (Leo et al. 1971; Hansch & Leo 1979)

4.15 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)

4.17 (shake flask-GC, Watarai et al. 1982)

4.17 (HPLC-k’ correlation, Hammers et al. 1982)

4.02 (generator column-GC/ECD, Miller et al. 1984; 1985)

4.18 (HPLC-RV correlation, Garst 1984)

4.31 (shake flask-GC, Chiou 1985)

4.49 (Hansch & Leo 1985)

4.32* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.31 (shake flask-GC, Pereira et al. 1988)

4.189 (slow stirring-GC, De Bruijn et al. 1989)

4.15 (recommended, Sangster 1993)

4.19 (recommended, Hansch et al. 1995)

4.34* ± 0.04 (shake flask-GC/ECD, Bahadur et al. 1997)

4.44 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.85 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

4.89* (20°C HPLC-k’ correlation, measured range 10–50°C, Su et al. 2002)

log K_{OA} = 68550/(2.303-RT) – 7.368; temp range 5–45°C (HPLC-k’ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF: at 25°C or as indicated

4.15 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.15–3.30 mean 3.26; 3.57–3.92 mean 3.61 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.34–4.67 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.26–3.61 (fish, Oliver 1984)
4.15 (guppy, female, 5.4% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
2.39–2.55 (fish, normalized, Tadokoro & Tomita 1987)
2.88 (fish, calculated-C<sub>d</sub>/C<sub>w</sub> or k<sub>1</sub>/k<sub>2</sub>, Connell & Hawker 1988; Hawker 1990)
4.32, 4.35, 4.38, 4.43 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
4.40, 4.45, 3.51, 4.22 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.26, 3.61; 3.48 (Oncorhynchus mykiss; Poecilia reticula, quoted lit., flow through conditions, Devillers et al. 1996)
2.68 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
3.26, 4.33; 3.271, 2.884 (quoted: whole fish, lipid content; calculated-MCI χ, K<sub>OC</sub>, Lu et al. 1999)
3.69; 3.64 (Oncorhynchus mykiss, wet wt. basis: quoted expl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K<sub>OC</sub>:
5.10; 4.20 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
2.85 (forest soil 0.2% OC, observed, Seip et al. 1986)
4.13 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
3.55 ± 0.47 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.69 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>½</sub>:
Volatilization: t<sub>½</sub> = 4.5 h from a model river of 1 m depth with water current 1 m/s and wind velocity 3 m/s at 20°C (Lyman et al. 1982).
Photolysis: may be susceptible to direct photolysis by sunlight (Howard 1989)
t<sub>½</sub> ~450 yr for sunlight photolysis at 40°N in the summer (Dulin et al. 1986)
k = 0.003 min<sup>−1</sup>, measured pseudo-first-order direct photolysis reaction with t<sub>½</sub> = (205.5 ± 7.5) min in aqueous solution (Peijnenburg et al. 1992)
Oxidation: rate constant k, for gas-phase second order rate constants, k<sub>OH</sub> for reaction with OH radical, k<sub>NO<sub>3</sub></sub> with NO<sub>3</sub> radical and k<sub>O<sub>3</sub></sub> with O<sub>3</sub> or as indicated, *data at other temperatures see reference:
k<sub>OH</sub> = 1.0 × 10<sup>–13</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
photooxidation t<sub>½</sub> = 6.17 months, based on a measured rate for the vapor phase reaction with photochemically produced hydroxyl radicals in air (Atkinson et al. 1985).
Hydrolysis: will not hydrolyze under normal environmental conditions (Howard 1989).
Biodegradation: resistant to biodegradation (Tabak et al. 1964; Howard 1989);
dechlorination pseudo-first order rate constant k = 0.069 d<sup>−1</sup> with t<sub>½</sub> = 10.1 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Biotransformation:
Bioconcentration Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:
k<sub>1</sub> = 8000 d<sup>−1</sup>; k<sub>2</sub> = 0.40 d<sup>−1</sup> (guppy, Königsmann & van Leeuwen 1980)
k<sub>1</sub> = 18.0 h<sup>−1</sup>; 1/k<sub>2</sub> = 60 h (guppy, quoted, Hawker & Connell 1985)
k<sub>1</sub> = 430 d<sup>−1</sup> (fish, quoted, Opperhuizen 1986)
log k<sub>1</sub> = 2.63 d<sup>−1</sup>; log k<sub>2</sub> = 0.440 d<sup>−1</sup> (fish, quoted, Connell & Hawker 1988)
log k<sub>1</sub> = 2.48 d<sup>−1</sup>; log k<sub>2</sub> = −0.40 d<sup>−1</sup> (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)
log k<sub>1</sub> = −0.40 d<sup>−1</sup> (fish, calculated-K<sub>OC</sub>, Thomann 1989)
k<sub>1</sub> = 7 mL g<sup>−1</sup> d<sup>−1</sup>, k<sub>2</sub> = 3 d<sup>−1</sup> (pond snail Lymnaea stagnalis, Legierse et al. 1998)

Half-Lives in the Environment:
Air: residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)
Surface Water: t<sub>½</sub> = 18 d under field conditions in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)
direct photolysis t<sub>½</sub> = 206 min in aqueous solution (Peijnenburg et al. 1992)
Groundwater:
Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:
Biota: biological half-lives, $t_{1/2} < 1$ d in trout, $t_{1/2} = 2$ d in sunfish and $t_{1/2} = 2$ d in guppy for trichlorobenzenes (Niimi 1987); $t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a).

### Table 6.1.1.7.1
Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,3,5-trichlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>log $K_{OW}$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC</td>
<td>shake flask-GC/ECD</td>
<td>shake flask-GC/ECD</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g \cdot m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>4.62</td>
<td>13</td>
</tr>
<tr>
<td>15</td>
<td>6.29</td>
<td>19</td>
</tr>
<tr>
<td>25</td>
<td>8.46</td>
<td>28</td>
</tr>
<tr>
<td>35</td>
<td>11.14</td>
<td>33</td>
</tr>
<tr>
<td>45</td>
<td>15.55</td>
<td>45</td>
</tr>
</tbody>
</table>

$\Delta H_{sol} = 22.04$ kJ/mol

$\Delta H/(kJ \cdot mol^{-1}) = -21.7$

$\Delta H/(kJ \cdot mol^{-1}) = -18.2$

$log K_{OW} = A - \frac{\Delta H}{2.303RT}$

$log K_{OA} = A + \frac{B}{2.303RT}$

$\Delta H_{OA}(kJ \cdot mol^{-1}) = 68.55$

$\Delta H = -18200$

$A = 1.1228$

$B = 68500$

**Figure 6.1.1.7.1** Logarithm of mole fraction solubility, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,3,5-trichlorobenzene.
Table 6.1.1.7.2
Reported vapor pressures of 1,3,5-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\cdot\log (T/K) \quad (4)
\end{align*}
\]

1. Stull 1947

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>63.8</td>
<td>666.6</td>
</tr>
<tr>
<td>78.0</td>
<td>1333</td>
</tr>
<tr>
<td>93.7</td>
<td>2666</td>
</tr>
<tr>
<td>110.8</td>
<td>5333</td>
</tr>
<tr>
<td>121.8</td>
<td>7999</td>
</tr>
<tr>
<td>136.0</td>
<td>13332</td>
</tr>
<tr>
<td>157.7</td>
<td>26664</td>
</tr>
<tr>
<td>183.0</td>
<td>53329</td>
</tr>
<tr>
<td>208.4</td>
<td>101325</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>eq. 1</td>
<td>P/µm</td>
</tr>
</tbody>
</table>

Sears & Hopke 1949

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>9–28°C</td>
<td>solid</td>
</tr>
<tr>
<td>A</td>
<td>12.176</td>
</tr>
<tr>
<td>B</td>
<td>2956.0</td>
</tr>
</tbody>
</table>

Rodebush gauge

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>63.5</td>
<td>measured between</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.29</td>
<td>1.493</td>
</tr>
<tr>
<td>0.29</td>
<td>1.383</td>
</tr>
<tr>
<td>10.31</td>
<td>4.492</td>
</tr>
<tr>
<td>10.31</td>
<td>4.556</td>
</tr>
<tr>
<td>20.25</td>
<td>12.41</td>
</tr>
<tr>
<td>20.25</td>
<td>12.40</td>
</tr>
<tr>
<td>30.15</td>
<td>34.58</td>
</tr>
<tr>
<td>30.15</td>
<td>34.56</td>
</tr>
<tr>
<td>40.09</td>
<td>83.96</td>
</tr>
<tr>
<td>40.09</td>
<td>83.89</td>
</tr>
<tr>
<td>50.09</td>
<td>193.4</td>
</tr>
<tr>
<td>60.13</td>
<td>442.4</td>
</tr>
<tr>
<td>25</td>
<td>20.44</td>
</tr>
</tbody>
</table>

Polednicek et al. 1996

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>P/µm</td>
<td></td>
</tr>
<tr>
<td>30.15</td>
<td>34.56</td>
</tr>
<tr>
<td>40.09</td>
<td>83.96</td>
</tr>
<tr>
<td>50.09</td>
<td>193.4</td>
</tr>
<tr>
<td>60.13</td>
<td>442.4</td>
</tr>
<tr>
<td>159.03</td>
<td>27045</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>solid</td>
<td></td>
</tr>
<tr>
<td>65.7</td>
<td>586</td>
</tr>
<tr>
<td>68.1</td>
<td>669</td>
</tr>
<tr>
<td>75.06</td>
<td>963</td>
</tr>
</tbody>
</table>

2. Blok et al. 2001

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>solid</td>
<td></td>
</tr>
<tr>
<td>series I</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>9–28°C</td>
<td>liquid</td>
</tr>
<tr>
<td>A</td>
<td>21.1215</td>
</tr>
<tr>
<td>B</td>
<td>3939.56</td>
</tr>
<tr>
<td>C</td>
<td>–71.2907</td>
</tr>
</tbody>
</table>
### TABLE 6.1.1.7.2 (Continued)

<table>
<thead>
<tr>
<th>Torsion, mass-loss effusion</th>
<th>Static-diaphragm manometer</th>
<th>Static-diaphragm manometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>-5.15</td>
<td>0.822</td>
<td>41.43</td>
</tr>
<tr>
<td>-3.65</td>
<td>0.984</td>
<td>44.47</td>
</tr>
<tr>
<td>-0.65</td>
<td>1.40</td>
<td>47.57</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>50.51</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>53.61</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.47</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.48</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>57.49</td>
</tr>
</tbody>
</table>

**FIGURE 6.1.1.7.2** Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trichlorobenzene.
6.1.1.8 1,2,3,4-Tetrachlorobenzene

Common Name: 1,2,3,4-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,3,4-tetrachlorobenzene
CAS Registry No: 634-66-2
Molecular Formula: C₆H₂Cl₄
Molecular Weight: 215.892

Melting Point (°C):
47.5 (Weast 1972–73; Lide 2003)

Boiling Point (°C):
254 (Lide 2003)

Density (g/cm³):

Molar Volume (cm³/mol):
142 (calculated-density, liquid molar volume, Chiou 1985)
179.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
17.0 (Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
16.95 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔHfus (kJ/mol):
17.0 (Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
16.95 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔSfus (J/mol K):
53.14 (Miller et al. 1984)

Fugacity Ratio at 25°C (assuming ΔSfus = 156 J/mol K), F: 0.602 (mp at 47.5°C)
0.608 (25°C, Suntio et al. 1988b)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
4.31 (shake flask-UV, Yalkowsky et al.)
3.42 (shake flask-GC, Koenemann 1981)
4.32 (recommended, Horvath 1982)
3.50 (22°C, Verschueren 1983)
12.2 (generator column-GC/ECD, Miller et al. 1984, 1985)
7.18 (23°C, shake flask-GC, Chiou 1985)
5.92 (shake flask-HPLC, Banerjee et al. 1984)
4.33 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
12.2 (generator column-GC, Doucette & Andren 1988)
3.27 (shake flask-GC/ECD, Kim & Saleh 1990)
12.0 (shake flask-GC, Boyd et al. 1998)
1.40, 2.11, 2.80, 5.25 (5, 15, 25, 35°C, estimated- RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (68.5°C, summary of literature data, temp range 68.5–254.0°C, Stull 1947)
8.76 (extrapolated-Antoine eq., supercooled liquid Pₛ, Weast 1972–73)
5.21 (calculated-Antoine eq. from Weast 1972–73, converted to solid Pₛ.; Mackay & Shiu 1981)
log (P/mmHg) = [−0.2185 × 12872.5/(T/K)] + 8.251056; temp range 68.5–254°C (Antoine eq., Weast 1972–73)
4.017, 3.49 (P_GC by GC-RT correlation with different GC columns, Bidleman 1984)
8.0 (supercooled liquid Pₛ, converted from literature Pₛ with ΔSfus, Bidleman 1984)
6.285 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
2.44 (supercooled liquid Pₛ, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log \( (P_L/\text{kPa}) = 5.7082 – 1517.2/(–117.384 + T/\text{K}) \); temp range 331–527 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

5.60 (selected, supercooled liquid \( P_L \), Suntio et al. 1988b; quoted, Ballschmiter & Wittlinger 1991)

8.0 (supercooled \( P_L \), converted from literature \( P_S \) with \( \Delta S_{\text{fus}} \), Hinckley et al. 1990)

4.02 (\( P_{\text{GC}} \) by GC-RT correlation, Hinckley et al. 1990)

12.1 (supercooled liquid \( P_L \), GC-Kovás retention indices correlation; Spieksma et al. 1994)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C or the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

70 (gas stripping-GC, Oliver 1985)

62.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

289 (modified EPICS method-GC, Ryu & Park 1999)

58.5 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

log \( K_{\text{AW}} \) = 5.014 – 1945/(T/\text{K}) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.:

4.72 (Leo et al. 1971)

4.46 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)

4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)

4.37 (shake flask-GC, Watarai et al. 1982)

4.94 (TLC-RT correlation, Bruggeman et al. 1982)

4.75 (shake flask-GC, Bruggeman et al. 1982)

4.41 (HPLC-k’ correlation, Hammers et al. 1982)

4.55 (generator column-GC, Miller et al. 1984)

4.60 (shake flask-GC, Chiu 1985)

4.65 (HPLC-RV/MS, Burkhard & Kuehl 1986)

4.61* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.60 (shake flask-GC, Pereira et al. 1988)

4.635 (shake flask/slow stirring-GC, De Bruijn et al. 1989)

4.54 (recommended, Sangster 1993)

4.64 (recommended, Hansch et al. 1995)

4.41 ± 0.06* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)

log \( K_{\text{OW}} \) = 0.6978 – 21100/[2.303·R(T/\text{K})], temp range 5–45°C (van’t Hoff eq. derived from lit. data, Bahadur et al. 1997)

4.30* (estimated RP-HPLC-k’ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \) at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

5.64*; 5.74 (generator column-GC; measured range –10 to 20°C, calculated, Harner & Mackay 1995)

log \( K_{\text{OA}} \) = –5.3 + 3254/(T/\text{K}); \( \Delta H_{\text{OA}} \) = 62.3 kJ/mol (Harner & Mackay 1995)

5.64 (calculated-S\text{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF at 25°C or as indicated:

4.86 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.25 (Briggs 1981)

3.36–3.75 mean 3.72; 4.00–4.15 mean 4.08 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.80–5.13 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.72–4.08 (fish, Oliver 1984)

3.70 (15°C, rainbow trout, Banerjee et al. 1984)

3.41–3.93 mean 3.80; 3.49–4.00 mean 3.91 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

3.72; .89 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)

3.38 (fathead minnow, Carlson & Kosian 1987)

4.9–5.4, 5.1: 4.1 (Niagara River plume, range, mean; calculated-\( K_{\text{OW}} \), Oliver 1987b)
4.70, 4.74, 4.75, 4.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
3.36 (guppy, Van Hoogan & Opperhuizen 1988)
5.46, 5.70, 4.68, 5.30 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.68; 3.79 (Scenedesmus spp. Coenobia, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
3.40 (guppy, steady-state conditions, rate const. ratio k₁/k₂, 96-h exposure, Sijm et al. 1993)
4.70 (guppy, lipid normalized BCF, Sijm et al. 1993)
3.72–4.08; 3.82 (Oncorhynchus mykiss; Poecilia reticulata, flow through conditions, Devillers et al. 1996)
3.89 (algae Selenastrum capricornutum, wet wt basis, isomer not specified, Wang et al. 1996)
4.28 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
3.96; 3.89 (Oncorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
3.49 (soil, sorption isotherm, converted from reported log K_{om} of 3.25, Briggs 1981)
3.27 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
3.16–4.42 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
5.00; 4.90 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
4.1–6.0, 5.2 (suspended sediment, average, Oliver 1987c)
3.52, 3.91, 3.75, 3.48, 3.52 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorilllite, sandy loam/allophone, clay loam/allophone, batch equilibrium-sorption isotherm, Kishi et al. 1990)
3.48–3.91 (soil, batch-equilibration, Kishi et al. 1990)
4.28 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
4.26 (sediment 3.86% OC, batch sorption equilibrium, Koelmans & Lijkelma 1992)
4.39 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)
3.70, 3.64, 3.84 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
4.14 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
3.25 (soil, sorption isotherm, shake flask-GC, soil organic matter, Briggs 1981)
4.90 (Niagara River-organic matter, Oliver & Charlton 1984)
4.90–5.40; 5.10; 4.10; 4.50 (Niagara-River plume: range; average; calculated-K_{OW}, algae > 50 μm, Oliver 1987b)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volutilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: dechlorination pseudo-first order rate constant k = 1.455 d⁻¹ with t_{1/2} = 0.5 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:
Biococoncentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
k₁ = 140 h⁻¹; k₂ = 0.021 h⁻¹ (rainbow trout, 15°C, Banerjee et al. 1984)
k₁ = 670 mL g⁻¹ d⁻¹; k₂ = 0.29 d⁻¹ (guppy, van Hoogan & Opperhuizen 1988)
k₁ = 670 ± 180 L kg⁻¹ d⁻¹; k₂ = 0.29 ± 0.06 d⁻¹ (guppies, 96-h exposure., Sijm et al. 1993)
k₁ = 1807.8 h⁻¹; k₂ = 0.304 h⁻¹ (algae Selenastrum capricornutum, isomer not specified, Wang et al. 1996)
k₁ = 141 mL g⁻¹ d⁻¹, k₂ = 1.5 d⁻¹ (pond snail Lymnaea stagnalis, Legierse et al. 1998)

Half-Lives in the Environment:
Air:
Surface Water:
Groundwater:
Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:
Biota: biological half-lives, $t_{1/2} = 3$ d in sunfish and $t_{1/2} = 2$ d in guppy for tetrachlorobenzenes (Niimi 1987); $t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a).

### TABLE 6.1.1.8.1
Reported vapor pressures and Henry’s law constants of 1,2,3,4-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor pressure (Pa)</th>
<th>Henry’s law constant (H/(Pa m³/mol))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\log P = A - B/(T/K)$</td>
<td>$\ln P = A - B/(T/K)$</td>
</tr>
<tr>
<td></td>
<td>$\log P = A - B/(C + t/°C)$</td>
<td>$\ln P = A - B/(C + t/°C)$</td>
</tr>
<tr>
<td></td>
<td>$\log P = A - B/(C + T/K)$</td>
<td>$\ln P = A - B/(C + T/K)$</td>
</tr>
<tr>
<td></td>
<td>$\log P = A - B/(T/K) - C\cdot\log (T/K)$</td>
<td>$\ln P = A - B/(T/K)$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stull 1947</th>
<th>ten Hulscher et al. 1992</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$P/(Pa)$</td>
<td>$H/(Pa \text{ m}^3/\text{mol})$</td>
</tr>
<tr>
<td>68.5</td>
<td>133.3</td>
<td>14.8</td>
</tr>
<tr>
<td>99.6</td>
<td>666.6</td>
<td>20.0</td>
</tr>
<tr>
<td>114.7</td>
<td>1333</td>
<td>20.1</td>
</tr>
<tr>
<td>131.2</td>
<td>2666</td>
<td>22.1</td>
</tr>
<tr>
<td>149.2</td>
<td>5333</td>
<td>24.1</td>
</tr>
<tr>
<td>160.0</td>
<td>7999</td>
<td>34.8</td>
</tr>
<tr>
<td>175.7</td>
<td>13332</td>
<td>50.0</td>
</tr>
<tr>
<td>198.0</td>
<td>26664</td>
<td>temp dependence eq.</td>
</tr>
<tr>
<td>225.5</td>
<td>53329</td>
<td>$\ln K_{AW} = A - B/(T/K)$</td>
</tr>
<tr>
<td>254.0</td>
<td>101325</td>
<td>A</td>
</tr>
<tr>
<td>46.5</td>
<td></td>
<td>B</td>
</tr>
</tbody>
</table>

$A = 22.156$,
$B = 5532.84$.
FIGURE 6.1.1.8.1 Logarithm of mole fraction solubility, vapor pressure and Henry’s law constant versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

TABLE 6.1.1.8.2
Reported octanol-water and octanol-air partition coefficients of 1,2,3,4-tetrachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Opperhuizen et al. 1988</th>
<th>log $K_{OW}$</th>
<th>Bahadur et al. 1997</th>
<th>log $K_{OW}$</th>
<th>Finizio &amp; Di Guardo 2001</th>
<th>log $K_{OW}$</th>
<th>Harner &amp; Mackay 1995</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC/ECD</td>
<td>t/°C $\log K_{OW}$</td>
<td>shake flask-GC/ECD</td>
<td>t/°C $\log K_{OW}$</td>
<td>GC-RT correlation</td>
<td>t/°C $\log K_{OW}$</td>
<td>generator column-GC</td>
<td>t/°C $\log K_{OA}$</td>
</tr>
<tr>
<td>13</td>
<td>4.83</td>
<td>19</td>
<td>4.61</td>
<td>28</td>
<td>4.37</td>
<td>33</td>
<td>4.66</td>
</tr>
<tr>
<td>15</td>
<td>4.65</td>
<td>25</td>
<td>4.41</td>
<td>35</td>
<td>4.28</td>
<td>45</td>
<td>4.15</td>
</tr>
<tr>
<td>ΔH/(kJ mol(^{-1})) = –26.3</td>
<td>enthalpy of transfer</td>
<td>ΔH/(kJ mol(^{-1})) = –21.1</td>
<td>log $K_{OW} = A - ΔH/2.303RT$</td>
<td>ΔH = –21100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>0.6978</td>
<td>A</td>
<td>-5.3</td>
<td>B</td>
<td>3254</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
**FIGURE 6.1.8.2** Logarithm of $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.
6.1.1.9 1,2,3,5-Tetrachlorobenzene

Common Name: 1,2,3,5-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,3,5-tetrachlorobenzene
CAS Registry No: 634-90-2
Molecular Formula: C₆H₂Cl₄
Molecular Weight: 215.892
Melting Point (°C):
  54.5  (Weast 1972–73; 1982–83; Lide 2003)
Boiling Point (°C):
  246  (Lide 2003)
Density (g/cm³):
  179.6  (calculated-Le Bas method at normal boiling point)
  141.0  (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
  19.0  (Miller et al. 1984; Chickos et al. 1999)
  19.32  (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔSfus (J/mol K):
  58.576  (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
  0.514 (mp at 54.5°C)
  0.556  (Suntio et al. 1988b)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  3.50  (shake flask-UV, Yalkowsky et al. 1979)
  4.02  (shake flask-LSC, Banerjee et al. 1980)
  4.11, 17.1  (LSC-¹⁴C, calculated-Kow, Veith et al. 1980)
  2.48  (shake flask-GC, Könemann 1981)
  3.51  (recommended, Horvath 1982)
  2.40  (22°C, Verschueren 1983)
  5.10  (shake flask-HPLC, Banerjee 1984)
  2.89  (generator column-GC/ECD, Miller et al. 1984, 1985)
  3.23  (shake flask-GC, Chiou 1985)
  3.46  (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
  4.32  (generator column-GC, Doucette & Andren 1988)
  4.32  (shake flask-GC/ECD, Kim & Saleh 1990)
  4.52  (shake flask-GC/ECD, Tam et al. 1996)
  3.44 ± 0.15*, 3.79 ± 0.23  (generator column-GC/ECD, shake flask-GC at 27°C, Shiu et al. 1997)
ln x = –4.4222 – 3162.74/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  133.3*  (58.2°C, summary of literature data, temp range 58.2–246°C, Stull 1947)
  18.6  (extrapolated-supercooled liquid PL, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 11982.1/(T/K)] + 7.925176; temp range 58.2–246°C (Antoine eq., Weast 1972–73)
  9.80  (solid PS, calculated from extrapolated vapor pressure PL with a fugacity ratio correction, Mackay & Shiu 1981)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics 1327

5.085 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
17.2; 9.56 (extrapolated-Antoine eq., supercooled liquid P_L, converted to P_S, Stephenson & Malanowski 1987)
\log(P_L/\text{kPa}) = 6.7756 - 2394/(–17.85 + T/K); temp range 331–519 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
15.1 (supercooled liquid P_L, GC-Kovás retention indices correlation; Spieksma et al. 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

159 (batch stripping-GC, Mackay & Shiu 1981)
99 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
160 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section.

4.50, 4.92 (shake flask-GC, HPLC-k′ correlation, Königemann et al. 1979)
4.46 (HPLC-RT correlation, Veith et al. 1979b)
4.46, 5.0 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
4.52 (shake flask-LSC, Banerjee et al. 1980)
5.05 (head-space GC, Hutchinson et al. 1980)
4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
4.56 (shake flask-GC, Watarai et al. 1982)
4.53 (HPLC-k′ correlation, Hammers et al. 1982)
4.51 (generator-column-GC/ECD, Miller et al. 1984; 1985)
4.61–4.73 (HPLC-RV correlation, Garst 1984)
4.59 (shake flask-GC, Chiou 1985)
4.59 (shake flask-GC, Pereira et al. 1988)
4.658 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
4.63 (recommended, Sangster 1993)
4.66 (recommended, Hansch et al. 1995)
4.55* ± –0.02 (shake flask-GC/ECD, Bahadur et al. 1997)
\log(K_{OW}) = 1.0159 – 20200/[2.303·R(T/K)]; temp range 5–45°C (van’t Hoff eq., Bahadur et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:

5.55 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
5.78* (20°C, HPLC-k′ correlation, measured range 10–50°C, Su et al. 2002)
\log(K_{OA}) = 66320/(2.303·RT) – 6.086; temp range 10–50°C (HPLC-k′ correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.26 (fathead minnow, Veith et al. 1979b)
4.86 (guppy-lipid basis, Königemann et al. 1979)
4.15, 4.86 (guppy-lipid basis, Königemann & van Leeuwen 1980)
3.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
3.46 (22°C, bluegill sunfish, Banerjee et al. 1984)
3.59 (fish, calculated-concentration ratio C_i/C_w or k_i/k_2, Connell & Hawker 1988; Hawker 1990)
4.73 (guppy-lipid phase, 12 to 31-d exposure studies, Gobas et al. 1989)
5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
3.64–4.89 (Poecilia reticulata, quoted lit., flow through conditions, Devillers et al. 1996)
3.89 (algae Selenastrum capricornutum, wet wt basis, isomer not specified, Wang et al. 1996)
4.27 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
4.11; 3.89 (Oncorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
3.20 (Koch 1983)
4.25 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
3.94 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)

Sorption Partition Coefficient, log $K_{OM}$:
3.20, 2.98 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k or Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Oxidation:
Hydrolysis:
Biodegradation: dechlorination pseudo-first order rate constant $k = 0.639 \, \text{d}^{-1}$ with $t_\frac{1}{2} = 1.1 \, \text{d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

\[
\begin{align*}
k_1 &= 15000 \, \text{d}^{-1}; \quad k_2 = 0.26 \, \text{d}^{-1} \quad \text{(guppy, Koenemann \& van Leeuwen 1980)} \\
k_1 &= 74 \, \text{h}^{-1}; \quad k_2 = 0.026 \, \text{h}^{-1} \quad \text{(bluegill sunfish, Banerjee et al. 1984)} \\
k_1 &= 33.8 \, \text{h}^{-1}; \quad 1/k_2 = 92.0 \, \text{h} \quad \text{(guppy, Hawker \& Connell 1985)} \\
k_1 &= 810 \, \text{d}^{-1} \quad \text{(fish quoted, Opperhuizen 1986)} \\
\log k_1 &= 2.91 \, \text{d}^{-1}; \quad \log 1/k_2 = -0.42 \, \text{d} \quad \text{(guppy, quoted, Connell \& Hawker 1988)} \\
\log k_1 &= 3.00 \, \text{d}^{-1}; \quad \log k_2 = -0.59 \, \text{d}^{-1} \quad \text{(guppy, 12 to 31-d exposure studies, Gobas et al. 1989)} \\
\log k_2 &= -0.58 \, \text{d}^{-1} \quad \text{(fish, calculated-KOW, Thomann 1989)} \\
k_1 &= 1807.8 \, \text{h}^{-1}; \quad k_2 = 0.304 \, \text{h}^{-1} \quad \text{(algae Selenastrum capricornutum, isomer not specified, Wang et al. 1996)} \\
k_1 &= 131 \, \text{mL g}^{-1} \, \text{d}^{-1}, \quad k_2 = 1.4 \, \text{d}^{-1} \quad \text{(pond snail Lymnaea stagnalis, Legierse et al. 1998)}
\end{align*}
\]

Half-Lives in the Environment:
Air:
Surface Water:
Groundwater:
Sediment: dechlorination $t_\frac{1}{2} = 1.8 \, \text{d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
Soil:
Biota: $t_\frac{1}{2} = 2–4 \, \text{d}$ in fish (Veith et al. 1980);
\[2 < t_\frac{1}{2} < 4 \, \text{d} \quad \text{in bluegill sunfish (Barrows et al. 1980)}.\]
TABLE 6.1.1.9.1
Reported aqueous solubilities, vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3,5-tetrachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log KOW</th>
<th>log KOA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-GC</td>
<td>summary of literature data</td>
<td>shake flask-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>5</td>
<td>1.7</td>
<td>58.2</td>
<td>133.3</td>
</tr>
<tr>
<td>15</td>
<td>2.43</td>
<td>89</td>
<td>666.6</td>
</tr>
<tr>
<td>25</td>
<td>3.44</td>
<td>104.1</td>
<td>1333</td>
</tr>
<tr>
<td>35</td>
<td>5.08</td>
<td>121.6</td>
<td>2666</td>
</tr>
<tr>
<td>45</td>
<td>7.03</td>
<td>140</td>
<td>5333</td>
</tr>
</tbody>
</table>

∆Hₜₗ = 26.3 kJ/mol

ΔH/(kJ mol⁻¹) = −20.2

log K⁰ = A + B/2.303RT

A | −6.086
B | 66320

m.p/°C | 54.5

FIGURE 6.1.1.9.1 Logarithm of mole fraction solubility, vapor pressure, K⁰ and K⁰ versus reciprocal temperature for 1,2,3,5-tetrachlorobenzene.
6.1.1.10 1,2,4,5-Tetrachlorobenzene

Common Name: 1,2,4,5-Tetrachlorobenzene
Synonym:
Chemical Name: 1,2,4,5-tetrachlorobenzene
CAS Registry No: 95-94-3
Molecular Formula: C₆H₂Cl₄
Molecular Weight: 215.892
Melting Point (°C):
- 139.5 (Lide 2003)
Boiling Point (°C):
- 244.5 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
- 116.2 (22°C, calculated-density)
- 179.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
- 23.64 (Miller et al. 1984)
Enthalpy of Fusion, ΔHfus (kJ/mol):
- 24.10 (Ruelle & Kesselring 1993; Chickos et al. 1999)
- 29.94 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔSfus (J/mol K):
- 58.576 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K.), F: 0.0753 (mp at 139.5°C)
- 0.073 (Suntio et al. 1988b)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.595 (shake flask-UV, Yalkowsky et al. 1979)
- 0.29 (shake flask-GC, Könemann 1981)
- 0.596 (recommended, Horvath 1982)
- 0.30 (22°C, quoted, Verschueren 1983)
- 2.35 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 0.465 (shake flask-HPLC, Banerjee 1984)
- 0.606 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
- 0.528* ± 0.018, 0.543 ± 0.016 (generator column-GC/ECD, shake flask-GC at 27°C, Shiu et al. 1997)
- 2.20 (shake flask-GC, Boyd et al. 1998)
In x = –4.529 – 3708.6/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 5333* (146.0°C, summary of literature data, temp range 146.0–245°C, Stull 1947)
- 10.1 (extrapolated-Antoine eq., supercooled liquid Pt, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 12828.8/(T/K)] + 8.282213; temp range 146–245°C (Antoine eq., Weast 1972–73)
- 0.72 (Pₜ converted from Pt of Weast 1972–73, Mackay & Shiu 1981)
- 0.20 (evaporation rate, Dobbs & Cull 1982)
- 2.163 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
2.98, 0.22 (supercooled liquid $P_L$, solid $P_S$, Stephenson & Malanowski 1987) 
log ($P/KPa$) = 9.1357 – 4642.36/(132.952 + T/K); temp range 419–518 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
7.497 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.615 (calculated-UNIFAC activity coefficients, Banerjee et al. 1990)
15.1; 12.5 (supercooled liquid $P_L$, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
0.392* (24.65°C, torsion, mass-loss effusion, measured range 17–32.5°C, Blok et al. 2001)

Henry’s Law Constant (Pa m^3/mol at 25°C):
101 (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.72 (Leo et al. 1971)
4.82, 4.56 (shake flask-GC, HPLC-$k'$ correlation, Könemann et al. 1979)
4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
4.46 (shake flask-GC, Watarai et al. 1982)
4.52 (HPLC-$k'$ correlation, Hammers et al. 1982)
4.51 (generator column-GC/ECD, Miller et al. 1984, 1985)
4.70 (shake flask-GC, Chiou 1985)
4.60 (HPLC-$k'$ correlation, Mailhot 1987)
5.16 (RP-HPLC-capacity factor correlation, Oppenhuizen & Voors 1987)
5.04 (slow stirring-GC, De Bruijn et al. 1989)
5.16 (calculated-fragment const., De Bruijn et al. 1989)
4.70 (shake flask-GC, Pereira et al. 1988)
4.63 (recommended, Sangster 1993)
4.70 (recommended, Hansch et al. 1995)
4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)
4.44* (estimated- RP-HPLC-$k'$ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:  
5.63*; 5.81 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
log $K_{OA}$ = –5.0 + 3176/(T/K); $\Delta H_{OA}$ = 60.8 kJ/mol (Harner & Mackay 1995)
5.62, 5.63 (calculated-S oct and vapor pressure P, quoted lit., Abraham et al. 2001)

Bioconcentration Factor, log $BCF$ at 25°C or as indicated:
0.20 (rats, adipose tissue, Geyer et al. 1980)
3.65 (fish, flowing water, Kenaga & Goring 1980; Kenaga)
3.36–3.79 mean 3.72; 4.04–4.18 mean 4.11 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
3.72–4.11 (fish, Oliver 1984)
2.80 (Tadokoro & Tomita 1987)
3.89 (green algae, Mailhot 1987)
4.08 (guppy, concn ratio of $C_{fish}/C_{water}$, Oppenhuizen & Voors 1987)
5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
2.76 (picea omorika, Reischl et al. 1989)
3.61, 4.70 (American flagfish: whole fish, fish lipid, Smith et al. 1990)
3.20 (fish, calculated, Figueroa & Simmons 1991)
3.72–4.11; 3.61 (Onkorhynchus mykiss; Jordanella floridae, quoted lit., flow through conditions, Devillers et al. 1996)
3.89 (algae Selenastrum capricornutum, wet wt basis, isomer not specified, Wang et al. 1996)
3.72, 4.80; 3.517, 3.417 (quoted: whole fish, lipid content; calculated-MCI $\chi$, calculated-$K_{OW}$, Lu et al. 1999)
3.89; 3.89 \textit{(Oncorhynchus mykiss}, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

\textbf{Sorption Partition Coefficient, log }K_{OC}:\]
\begin{itemize}
\item 3.20 \textit{(Kenaga 1980a)}
\item 3.49 \textit{(soil, sorption isotherm, converted from reported log }K_{OM}\textit{ of 3.25, Briggs 1981)}
\item 3.36 \textit{(river sediment, 0.56\% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)}
\item 3.24–4.50 \textit{(five soils, 0.04–0.73\% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)}
\item 5.10; 4.70 \textit{(field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)}
\item 2.79 \textit{(McLaurin sandy loam, OC 0.66\%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)}
\item 3.94 ± 0.33 \textit{(suspended particulates in coastal waters, Masunaga et al. 1996)}
\item 3.48 \textit{(soil: organic carbon OC ≥ 0.1\%, average, Delle Site 2001)}
\end{itemize}

\textbf{Environmental Fate Rate Constants, }k\textbf{ or Half-Lives, }t_{1/2};\]
\begin{itemize}
\item \textbf{Volatileization:}
\item \textbf{Photolysis:}
\item Oxidation: \(t_{1/2} = 763.1–7631\text{ h, based on photooxidation half-life in air (Howard et al. 1991)}\)
\item Hydrolysis: base rate constant \(k < 0.9 \text{ M}^{-1}\text{ h}^{-1}\text{ at 25°C with a calculated }t_{1/2} > 900 \text{ yr at pH 7, based on assumed bases mediated 1\% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)}\)
\item first order hydrolysis \(t_{1/2} > 879 \text{ yr (Howard et al. 1991)}\)
\item Biodegradation: \(t_{1/2}(\text{aerobic}) = 672–4320\text{ h, based on unacclimated aerobic screening test data; }t_{1/2}(\text{anaerobic}) = 2880–17280\text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\)
\item dechlorination pseudo-first order \(k = 0.037 \text{ d}^{-1}\text{ with }t_{1/2} = 18.7\text{ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)}\).
\item \textbf{Biotransformation:}
\item Bioconcentration, Uptake \((k_1)\text{ and Elimination }\(k_2\text{ Rate Constants:}\)
\item \(k_1 = 1490 \text{ mL g}^{-1}\text{ d}^{-1}; k_2 = 0.14 \text{ d}^{-1}\text{ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)}\)
\item \(k_1 = 1630 \text{ d}^{-1}; 171000 \text{ d}^{-1}; k_2 = 0.4 \text{ d}^{-1}, 0.34 \text{ d}^{-1}\text{ (American flagfish: whole fish, fish lipid, Smith et al. 1990)}\)
\item \(k_1 = 0.4 \text{ d}^{-1}, 2.35 \text{ d}^{-1}\text{ (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)}\)
\item \(k_1 = 1807.8 \text{ h}^{-1}; k_2 = 0.304 \text{ h}^{-1}\text{ (algae }Selenastrum capricornutum,\text{ isomer not specified, Wang et al. 1996)}\)
\item \textbf{Half-Lives in the Environment:}
\item Air: \(t_{1/2} = 763.1–7631\text{ h, based on photooxidation half-life in air (Howard et al. 1991)}\)
\item Surface Water: hydrolysis \(t_{1/2} > 900 \text{ yr at pH 7 and 25°C (Ellington et al. 1988)}\)
\item \(t_{1/2} = 672–4320\text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\)
\item Groundwater: \(t_{1/2} = 1344–8640\text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\)
\item Sediment: dechlorination \(t_{1/2} = 18.7\text{ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)}\).
\item Soil: \(t_{1/2} = 672–4320\text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\)
\item Biota: \(t_{1/2} < 5\text{ d in worms at 8°C (Oliver 1987a); biological }t_{1/2} = 3\text{ d in sunfish, }t_{1/2} = 2\text{ d in guppy for tetrachlorobenzenes (Niimi 1987)};\)
\item \(t_{1/2} = 33\text{ d in }Picea omorika\text{ (Reischl et al. 1989); }t_{1/2} = 1.72\text{ d clearance from American flagfish (Smith et al. 1990);}\)
\item elimination \(t_{1/2} = 2.01\text{ d from earthworm in water (Belfroid et al. 1993); elimination }t_{1/2} = 0.204\text{ d and 2.63 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994).}\)
TABLE 6.1.1.10.1
Reported aqueous solubilities and vapor pressures of 1,2,4,5-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-GC</td>
<td>summary of literature data</td>
<td>torsion, mass loss effusion</td>
<td>static-diaphragm manometer</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>5</td>
<td>0.298</td>
<td>146.0</td>
<td>5333</td>
<td>16.85</td>
</tr>
<tr>
<td>15</td>
<td>0.322</td>
<td>157.7</td>
<td>7999</td>
<td>19.45</td>
</tr>
<tr>
<td>25</td>
<td>0.528</td>
<td>173</td>
<td>13332</td>
<td>22.05</td>
</tr>
<tr>
<td>35</td>
<td>0.739</td>
<td>196</td>
<td>26664</td>
<td>24.65</td>
</tr>
<tr>
<td>45</td>
<td>1.127</td>
<td>220.5</td>
<td>53329</td>
<td>27.25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>245</td>
<td>101325</td>
<td>29.85</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{sol}} = 30.8 \text{ kJ/mol} \]

\[ \mp = 129.82 \]

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 82.10 \]

at 353 K

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 132.79 \]

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 2770 \]

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 136.82 \]

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 3500 \]

FIGURE 6.1.1.10.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.
### TABLE 6.1.1.10.2
Reported octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4,5-tetrachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log $K_{OW}$</th>
<th>t/°C</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4.63</td>
<td>25</td>
<td>5.63</td>
</tr>
<tr>
<td>15</td>
<td>4.54</td>
<td>–10</td>
<td>7.056</td>
</tr>
<tr>
<td>25</td>
<td>4.44</td>
<td>0</td>
<td>6.622</td>
</tr>
<tr>
<td>35</td>
<td>4.26</td>
<td>9.88</td>
<td>6.204</td>
</tr>
</tbody>
</table>

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 60.8$

$\log K_{OA} = A + B/T$

- A = –5.0
- B = 3176

### FIGURE 6.1.1.10.2
Logarithm of $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.
### Pentachlorobenzene

**Chemical Name:** Pentachlorobenzene  
**CAS Registry No:** 608-93-5  
**Molecular Formula:** C₆HCl₅  
**Molecular Weight:** 250.337  

**Melting Point (°C):**  
86  
(Weast 1972–73; Lide 2003)

**Boiling Point (°C):**  
277  
(Weast 1972–72; Lide 2003)

**Density (g/cm³ at 20°C):**  
1.8342  
(16.5°C, Weast 1972–73; Horvath 1982)

**Molar Volume (cm³/mol):**  
136.5  
(16.5°C, calculated-density, Weast 1972–73; Horvath 1982)  
166  
(liquid molar volume, Chiou 1985)  
200.5  
(calculated-Le Bas method at normal boiling point)

**Enthalpy of Vaporization, ∆HV (kJ/mol):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.585</td>
<td>(Miller et al. 1984)</td>
</tr>
<tr>
<td>20.60</td>
<td>(Ruelle et al. 1993; Chickos et al. 1999)</td>
</tr>
<tr>
<td>20.1</td>
<td>(Ruelle &amp; Kesselring 1997)</td>
</tr>
</tbody>
</table>

**Enthalpy of Fusion, ∆Hfus (kJ/mol):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.585</td>
<td>(Miller et al. 1984)</td>
</tr>
<tr>
<td>20.60</td>
<td>(Ruelle et al. 1993; Chickos et al. 1999)</td>
</tr>
<tr>
<td>20.1</td>
<td>(Ruelle &amp; Kesselring 1997)</td>
</tr>
</tbody>
</table>

**Entropy of Fusion, ∆Sfus (J/mol K):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>57.74</td>
<td>(Miller et al. 1984)</td>
</tr>
</tbody>
</table>

**Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K.), F:** 0.252  
(mp at 86°C)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.56</td>
<td>(shake flask-UV, Yalkowsky et al. 1979)</td>
</tr>
<tr>
<td>1.33</td>
<td>(shake flask-LSC, Banerjee et al. 1980)</td>
</tr>
<tr>
<td>0.135</td>
<td>(Kenaga &amp; Goring 1980; Kenaga 1980a)</td>
</tr>
<tr>
<td>1.34</td>
<td>(shake flask-LSC-¹³C, Veith et al. 1980)</td>
</tr>
<tr>
<td>0.24</td>
<td>(shake flask-GC, Koenemann 1981)</td>
</tr>
<tr>
<td>0.562</td>
<td>(recommended, Horvath 1982)</td>
</tr>
<tr>
<td>0.831</td>
<td>(generator column-GC/ECD, Miller et al. 1984, 1985)</td>
</tr>
<tr>
<td>0.385</td>
<td>(23°C, shake flask-GC, Chiou 1985)</td>
</tr>
<tr>
<td>0.180</td>
<td>(generator column-GC/ECD, Opperhuizen et al. 1985)</td>
</tr>
<tr>
<td>0.552</td>
<td>(recommended, IUPAC Solubility Data Series, Horvath &amp; Getzen 1985)</td>
</tr>
<tr>
<td>3.46</td>
<td>(calculated-Kow and HPLC-RT correlation, Chin et al. 1986)</td>
</tr>
<tr>
<td>0.419* ± 0.018, 0.447 ± 0.014</td>
<td>(generator column-GC/ECD, shake flask-GC/ECD at 27°C, Shiu et al. 1997)</td>
</tr>
<tr>
<td>0.87</td>
<td>(shake flask-GC, Boyd et al. 1998)</td>
</tr>
</tbody>
</table>

ln x = −3.61482 − 4093.10/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

2.75, 3.50  
(supercritical fluid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>133*</td>
<td>(98.6°C, summary of literature data, temp range 98.6–276°C, Stull 1947)</td>
</tr>
</tbody>
</table>
0.889  (extrapolated-Antoine eq., supercooled liquid $P_L$, Weast 1972–73)
0.219  ($P_S$ calculated from $P_L$ of Weast 1972–73; Mackay & Shiu 1981)

$\log (P/mmHg) = \left[\frac{0.2185 \times 15124.2}{(T/K)} + 8.90797\right]$; temp range 98.6–276°C (Antoine eq., Weast 1972–73)
1.44  (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
1.08, 0.28  (supercooled liquid $P_L$, solid $P_S$, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/kPa) = 8.00795 – 3325.33/(4.814 + T/K)$; temp range 371–549 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

1.718  (GC-RT correlation, Watanabe & Tatsukawa 1989)
2.49, 2.19  (supercooled liquid $P_L$, GC-Kovás retention indices correlation; quoted lit., Spieksma et al. 1994)
0.212, 0.39* (25°C extrapolated; 30.3°C, static method-pressure gauge, measured range 30.3–179°C, Polednicek et al. 1996)

$\ln (P_S/Pa) = 30.4445 – 8654.67/[(T/K) – 27.6534]$; temp range 303.45–353.17 K (solid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)

$\ln (P_L/Pa) = 23.4783 – 6188.33/[(T/K) – 34.6922]$; temp range 365–452 K (liquid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)

$\log (P/kPa) = 15.6174 – 4831.4/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C or reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

71.9  (gas stripping-GC, Oliver 1985)
59.0*  (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)
52.6  (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 5.607 – 2132/(T/K)$ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

74, 70 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

5.79  (calculated-fragment const., Yalkowsky et al. 1979)
4.88, 5.52  (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979)
4.94  (shake flask-LSC, Banerjee et al. 1980)
4.94, 5.29  (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
5.17  (shake flask-GC, Watarai et al. 1982)
5.06  (HPLC-k′ correlation, Hammers et al. 1982)
5.69  (HPLC-RT correlation, Bruggeman et al. 1982)
5.03  (generator column-GC/ECD, Miller et al. 1984; 1985)
5.17  (shake flask-HPLC, Banerjee 1984)
5.11–5.21  (HPLC-RV correlation, Garst 1984)
5.20  (shake flask-GC, Chiou 1985)
4.97  (calculated-$K_{OW}$ and HPLC-RT correlation, Chin et al. 1986)
6.12  (HPLC-k′ correlation, De Kock & Lord 1987)
5.47  (HPLC-RT correlation, Doucette & Andren 1988)
5.20  (shake flask-GC, Pereira et al. 1988)
5.05*  (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
5.183  (shake flask/slow stirring-GC, De Bruijn et al. 1989)
5.17  (recommended, Sangster 1993)
5.18  (recommended, Hansch et al. 1995)
4.94* ± 0.03  (shake flask-GC/ECD, Bahadur et al. 1997)
log $K_{OW} = 0.9255 - 22800/(T/K)$; temp range 5–45°C (van’t Hoff eq., Bahadur et al. 1997)

5.67–5.78 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)

5.08, 5.19 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

$6.27^*; 6.46$ (generator column-GC, measured range –10 to 20°C, calculated, Harner & Mackay 1995)

$7.93, 7.418, 6.539$ (–10, 0, 10, 18.7°C, generator column-GC, Harner & Mackay 1995)

log $K_{OA} = -6.2 + 3722.3/(T/K)$; temp range –10 to 20°C, $\Delta H_{OA} = 72.3$ kJ/mol (generator column-GC, Harner & Mackay 1995)

6.50 (calculated-$K_{OW}/K_{AW}$, Wania & Mackay 1996)

6.49, 6.27 (calculated-$S_{oct}$ and vapor pressure $P$, quoted lit., Abraham et al. 2001)

6.90, 6.73 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.89 (trout muscle, Neely et al. 1974)

3.70 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)

5.40 (guppy, lipid content, Königsmann et al. 1979)

3.53 (bluegill sunfish, Veith et al. 1980)

5.33 (bluegill sunfish, whole body, flow system, Barrows 1980)

5.41 (guppy, lipid basis, Königsmann & van Leeuwen 1980)

3.84 (fish, flowing water, Garten & Trabalka 1983)

3.46–4.15 mean 4.11; 4.26–4.36 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

5.19–5.36 (rainbow trout, lipid basis, Oliver & Niimi 1983)

4.11–4.30 (rainbow trout, Oliver 1984)

3.71 (22°C, bluegill sunfish, 1.5% lipid, Banerjee et al. 1984)

3.65; 3.86 (15°C, rainbow trout, 1.8% lipid; guppy, 2.8% lipid, Banerjee et al. 1984)

3.60; 3.49 (algae: exp.; calculated, Geyer et al. 1984)

3.65 (algae, Freitag et al. 1984; Halgon & Reggiani 1986)

3.48 (fish, Freitag et al. 1984; Halgon & Reggiani 1986)

3.48, 3.65, 4.16 (fish, algae, activated sludge, Freitag et al. 1985)

4.23 (guppy, calculated-rate constants ratio $k_1/k_2$, Oppenhuizen et al. 1985)

3.92 (fathead minnow, Carlson & Kosian 1987)

2.83, 2.65 (human fat, Geyer et al. 1987)

4.28, 4.30 (worm, fish, Oliver 1987a)

3.36–3.42 (fish, Tadokoro & Tomita 1987)

5.46 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1989)

3.87 (picea omorika, Reischl et al. 1989)

5.33 (fish, calculated-$K_{OW}$, Thomann 1989)

4.14, 2.96, 4.23 (fish, Connell & Hawker 1988; Hawker 1990)

5.11, 5.18, 5.20, 5.28 (13, 19, 28, 33°C, female guppy, Oppenhuizen et al. 1988)

3.67 (guppy, Van Hoogan & Oppenhuizen 1988)

5.93, 6.12, 4.96, 5.57 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)

4.22 (Scenedesmus spp. Coenobia, dry wt., batch adsorption, Koelmans et al. 1993)

3.70 (guppy, steady-state conditions, rate const. ratio $k_1/k_2$, 96-h exposure, Sijm et al. 1993)

5.00 (guppy, lipid normalized BCF, Sijm et al. 1993)

4.11–4.30; 2.94–4.36; 3.53 (Oncorhynchus mykiss; Poecilia reticulata; Lepomis macrochirus, quoted lit., flow through conditions, Devillers et al. 1996)

5.22–5.50 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)

4.11, 5.19; 3.797, 3.877 (quoted: whole fish, lipid content; calculated-MCI $\chi$, calculated-$K_{OW}$, Lu et al. 1999)

4.09; 3.96 (Oncorhynchus mykiss, wet wt. basis: quoted exp.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)
Sorption Partition Coefficient, $\log K_{OC}$:

- 4.11 (Kenaga 1980a)
- 5.30, 5.40 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
- 4.60 (bottom sediment, Karickhoff & Morris 1985)
- 4.9–6.2, 5.8 (suspended sediment, average, Oliver 1987c)
- 5.7 (algae > 50 µm, Oliver 1987c)
- 5.50–5.90, 5.70 (Niagara River plume: range, average, Oliver 1987b)
- 4.49 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
- 4.68 (lake sediment 2.5% OC, batch sorption equilibrium, Schrap et al. 1994)
- 4.59 ± 0.41 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 4.91 (sediment: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 1088–10877$ h, based on estimated rate constant for the vapor phase reaction with OH radicals in air (Howard et al. 1991)

Hydrolysis: base rate constant $k < 0.9$ M$^{-1}$ h$^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first order $t_{1/2} > 879$ yr (Howard et al. 1991)

Biodegradation: $t_{1/2}$ (aerobic) = 4656–8280 h, based on estimated unacclimated aerobic soil grab sample data; $t_{1/2}$ (anaerobic) = 18642–33120 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

dechlorination pseudo-first order rate constant $k = 0.557$ d$^{-1}$ with $t_{1/2} = 1.2$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 18.76$ h$^{-1}$; $k_2 = 0.00238$ h$^{-1}$ (trout, Neely et al. 1974)
- $k_1 = 22000$ d$^{-1}$; $k_2 = 0.14$ d$^{-1}$ (guppy, Konemann & van Leeuwen 1980)
- $k_1 = 130$ d$^{-1}$; $k_2 = 0.15$ d$^{-1}$ (guppy, Bruggeman et al. 1984)
- $k_1 = 110$ h$^{-1}$; $k_2 = 0.021$ h$^{-1}$ (22°C, bluegill sunfish, Banerjee et al. 1984)
- $k_1 = 170$ h$^{-1}$; $k_2 = 0.036$ h$^{-1}$ (15°C, rainbow trout, Banerjee et al. 1984)
- $k_1 = 98$ h$^{-1}$; $k_2 = 0.014$ h$^{-1}$ (15°C, guppy, Banerjee et al. 1984)
- $k_1 = 5.4$ h$^{-1}$; $1/k_2 = 0.160$ h (guppy, quoted, Hawker & Connell 1985)
- $k_1 = 1400$ d$^{-1}$; $k_2 = 0.078$ d$^{-1}$ (guppy, Opperhuizen et al. 1985)
- $k_1 = 1200$ d$^{-1}$ (fish, quoted, Opperhuizen 1986)
- $k_2 = 0.00309$, 0.00402 d$^{-1}$ (rainbow trout, calc-fish mean body weight, Barber et al. 1988)
- log $k_1 = 3.08$ d$^{-1}$; log $1/k_2 = 0.96$ d (fish, quoted, Connell & Hawker 1988)
- $k_1 = 0.049$ h$^{-1}$; $k_2 = 0.027$ h$^{-1}$ (mayfly-sediment model II, Gobas et al. 1989b)
- log $k_1 = -0.82$ d$^{-1}$; $-0.96$ d$^{-1}$ (fish, calculated-$K_{ow}$, Thomann 1989)
- $1/k_2 = 0.12$, 12.9 d (guppy, Clark et al. 1990)
- $k_1 = 710$ ± 290 L kg$^{-1}$ d$^{-1}$; $k_2 = 0.15$ ± 0.04 d$^{-1}$ (guppies, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: $t_{1/2} = 1088–10877$ h, based on estimated rate constant for the vapor phase reaction with OH radicals (Howard et al. 1991)

Surface Water: $t_{1/2} = 4656–8280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater: $t_{1/2} = 9312–16560$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment: dechlorination $t_{1/2} = 1.20$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil: $t_{1/2} = 4656$–$8280$ h, based on estimated unacclimated aerobic soil grab sample data (Howard et al. 1991).

Biota:
- $t_{1/2} > 7$ d in fish (Veith et al. 1980);
- $t_{1/2} > 7$ d in bluegill sunfish (Barrows et al. 1980);
- $t_{1/2} = 4.6$ d in guppy (Bruggeman et al. 1984);
- $t_{1/2} = 8.9$ d in guppy (Opperhuizen et al. 1985);
- $t_{1/2} < 5$ d in worms at $8°C$ (Oliver 1987a);
- biological half-lives, $t_{1/2} > 7$ d in sunfish, $t_{1/2} = 4, 5$ and $< 5$ d in guppy (Niimi 1987);
- $t_{1/2} = 27$ d in *Picea omorika* (Reischl et al. 1989);
- elimination $t_{1/2} = 5.46$ d from earthworm in water (Belfroid et al. 1993);
- elimination $t_{1/2} = 0.53$ d and $5.9$ d in a two-phase kinetics from earthworm in OECD soil (Belfroid et al. 1994);
- elimination $t_{1/2} = 0.60$ d from earthworm in Volgermeerpolder soil (Belfroid et al. 1995).

### TABLE 6.1.1.11.1
Reported aqueous solubilities of pentachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Shiu et al. 1997</th>
<th>generator column-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$S/g \cdot m^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>0.145</td>
</tr>
<tr>
<td>15</td>
<td>0.254</td>
</tr>
<tr>
<td>25</td>
<td>0.419</td>
</tr>
<tr>
<td>35</td>
<td>0.618</td>
</tr>
<tr>
<td>45</td>
<td>0.856</td>
</tr>
<tr>
<td>shake flask-GC</td>
<td>27</td>
</tr>
</tbody>
</table>

### TABLE 6.1.1.11.2
Reported vapor pressures of pentachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

1. **Stull 1947**

<table>
<thead>
<tr>
<th>summary of lit. data</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
</tr>
<tr>
<td>98.6</td>
</tr>
<tr>
<td>129.7</td>
</tr>
<tr>
<td>144.3</td>
</tr>
<tr>
<td>160</td>
</tr>
<tr>
<td>178.5</td>
</tr>
</tbody>
</table>

2. **Polednicek et al. 1996**

| P/Pa | $T/K$ | $P/Pa$ |
| solid | liquid |
| 30.3 | 0.385 | 98.65 | 167.99 |
| 30.3 | 0.401 | 98.69 | 167.56 |
| 40.26 | 1.163 | 108.65 | 285.2 |
| 40.27 | 1.167 | 108.68 | 284.76 |
| 50.27 | 3.227 | 118.82 | 470.83 |

3. **Roháč et al. 1999**

<table>
<thead>
<tr>
<th>recommended</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T/K$</td>
</tr>
<tr>
<td>233.15</td>
</tr>
<tr>
<td>243.15</td>
</tr>
<tr>
<td>253.15</td>
</tr>
<tr>
<td>263.15</td>
</tr>
<tr>
<td>273.15</td>
</tr>
</tbody>
</table>

(Continued)
### TABLE 6.1.11.2 (Continued)

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Polednicek et al. 1996</th>
<th>Roháč et al. 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>summary of lit. data</strong></td>
<td><strong>pressure gauge</strong></td>
<td><strong>recommended</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( P/Pa )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>190.1</td>
<td>7999</td>
<td>50.27</td>
</tr>
<tr>
<td>205.5</td>
<td>13332</td>
<td>60.14</td>
</tr>
<tr>
<td>227</td>
<td>26664</td>
<td>60.16</td>
</tr>
<tr>
<td>251.5</td>
<td>53329</td>
<td>70.05</td>
</tr>
<tr>
<td>276</td>
<td>101325</td>
<td>70.05</td>
</tr>
<tr>
<td>80.02</td>
<td>47.29</td>
<td>159.06</td>
</tr>
</tbody>
</table>

\( \text{mp/°C} \) 85.5

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( T/K )</th>
<th>( P/Pa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### 2.

**Roháč et al. 1999**

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>( P/Pa )</th>
<th>continued</th>
<th>T/K</th>
<th>( P/Pa )</th>
<th>( T/K )</th>
<th>( P/Pa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>363.15</td>
<td>97.5</td>
<td>liquid</td>
<td>473.15</td>
<td>11440</td>
<td>Cox eq.</td>
<td></td>
</tr>
<tr>
<td>373.15</td>
<td>173.9</td>
<td>483.15</td>
<td>15500</td>
<td>eq. 5</td>
<td>P/Pa</td>
<td></td>
</tr>
<tr>
<td>383.15</td>
<td>298.8</td>
<td>493.15</td>
<td>20700</td>
<td>( A_0 )</td>
<td>3.419638</td>
<td></td>
</tr>
<tr>
<td>393.15</td>
<td>486.4</td>
<td>503.15</td>
<td>27250</td>
<td>( 10^3 A_1 )</td>
<td>(-1.1673259 )</td>
<td></td>
</tr>
<tr>
<td>403.15</td>
<td>799.8</td>
<td>513.15</td>
<td>35430</td>
<td>( 10^7 A_2 )</td>
<td>7.7842905</td>
<td></td>
</tr>
<tr>
<td>413.15</td>
<td>1253</td>
<td>523.15</td>
<td>45510</td>
<td>T/K</td>
<td>357.0</td>
<td></td>
</tr>
<tr>
<td>423.15</td>
<td>1912</td>
<td>533.15</td>
<td>57820</td>
<td>P/Pa</td>
<td>67.0</td>
<td></td>
</tr>
<tr>
<td>433.15</td>
<td>2848</td>
<td>543.15</td>
<td>72710</td>
<td>bp/K</td>
<td>558.42</td>
<td></td>
</tr>
<tr>
<td>443.15</td>
<td>4151</td>
<td>553.15</td>
<td>90570</td>
<td>for temp range 365–452 K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>453.15</td>
<td>5927</td>
<td>563.15</td>
<td>111800</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>463.15</td>
<td>8306</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 6.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for pentachlorobenzene.

TABLE 6.1.1.11.3
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of pentachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log $K_{OW}$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-GC</td>
<td>shake flask-GC/ECD</td>
<td>shake flask-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
</tr>
<tr>
<td>14.8</td>
<td>37.4</td>
<td>13</td>
</tr>
<tr>
<td>20</td>
<td>59.0</td>
<td>19</td>
</tr>
<tr>
<td>20.1</td>
<td>49.4</td>
<td>28</td>
</tr>
<tr>
<td>22.1</td>
<td>68.1</td>
<td>33</td>
</tr>
<tr>
<td>24.1</td>
<td>66.7</td>
<td>45</td>
</tr>
<tr>
<td>34.8</td>
<td>124.1</td>
<td></td>
</tr>
<tr>
<td>50.5</td>
<td>276.2</td>
<td>ΔH/(kJ mol⁻¹) = –30.8</td>
</tr>
</tbody>
</table>

Log $K_{OW}$ = A – B/(T/K)

H/(Pa m³/mol) = 21.4142

A = 21.4142

B = 5108

© 2006 by Taylor & Francis Group, LLC
FIGURE 6.1.11.2 Logarithm of Henry’s law constant, $K_{OW}$ and $K_{OA}$ versus reciprocal temperature for pentachlorobenzene.
6.1.1.12 Hexachlorobenzene

Common Name: Hexachlorobenzene
Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin’s carbon chloride
Chemical Name: hexachlorobenzene
CAS Registry No: 118-74-1
Molecular Formula: C₆Cl₆
Molecular Weight: 284.782

Melting Point (°C):
228.83 (Lide 2003)

Boiling Point (°C):
325 (Lide 2003)

Density (g/cm³ at 20°C):
1.5691 (23.6°C, Weast 1972–73; Horvath 1982)
2.004 (23°C, Lide 2003)

Molar Volume (cm³/mol):
181.5 (23.6°C, calculated-density, Weast 1972–73; Horvath 1982)
221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
23.85 (Plato & Glasgow 1969; Ruelle et al. 1993; Chickos et al. 1999)
28.74 (Tsonopoulos & Prausnitz 1971)
22.40 (Miller et al. 1984)

Entropy of Fusion, ΔSfus (J/mol K):
57.32 (Tsonopoulos & Prausnitz 1971)
44.77 (Miller et al. 1984)
47.1 (Hinckley et al. 1990; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.01 (mp at 228.83°C)
0.009 (Miller et al. 1985; Suntio et al. 1988b)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.005 (generator column-GC/ECD, Weil et al. 1974)
0.006 (shake flask-LSC/¹⁴C, Lu & Metcalf 1975)
0.11 (shake flask-nephelometric spectrophotofluorometry, Hollifield 1979)
0.005 (shake flask-UV, Yalkowsky et al. 1979)
0.0039 (shake flask-GC, Könemann 1981)
0.00921, 0.00996 (15, 25°C, generator column/elution method, average values of 6–7 labs., OECD 1981)
0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)
0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)
0.09 (recommended, Horvath 1982)
0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.005 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
0.00544* ± 0.00018 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
0.38 (generator column-GC, Boyd et al. 1998)
0.0050 ± 0.00002 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

log [Sₜ/(mol/L)] = 0.450 – 1212/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = −8.22956 – 4037.26/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.010* (generator column-GC/ECD, measured range 15–55°C, Oleszek-Kudlak et al. 2004)

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
0.0273, 0.398 (supercooled liquid: derivation of literature-derived value FAV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* (114.1°C, summary of literature data, temp range 114.1–309.4°C, Stull 1947)
- 0.00028 (extrapolated from Antoine eq., Sears & Hopke 1949)
- \( \log(P/mmHg) = 11.397 - \frac{4197.3}{(T/K)} \); temp range 96–124°C (Rodebush gauge, Sears & Hopke 1949)
- \( \log(P/mmHg) = \left[ -0.2185 \times 15199.1/(T/K) \right] + 8.550497 \); temp range 114.4–309.4°C (Antoine eq., Weast 1972–73)
- 0.0015 (Callahan et al. 1979)
- 0.0026 (OECD 1979)
- 0.00145 (20°C, Kiltzer et al. 1979)
- 0.0023* (gas saturation, measured range 15–45°C, Farmer et al. 1980)
- \( \log(P/mmHg) = 12.94 - \frac{5279}{(T/K)} \); temp range 15–45°C (gas saturation, Farmer et al. 1980)
- 0.000453; 0.000167 (Klein et al. 1981)
- 0.0019* (gas saturation, measured range 10–50°C, OECD 1981)
- \( \log(P/mmHg) = 12.237 - \frac{5152.1}{(T/K)} \); temp range 10–50°C (gas saturation, OECD 1981)
- 0.00046 (evaporation rate, Dobbs & Cull 1982)
- 0.00121 (extrapolated-Antoine eq., Gückel et al. 1982)
- 0.0006 (20°C, evaporation rate and gravimetric method, Gückel et al. 1982)
- 0.159, 0.122 (P_{ gc } by GC-RT correlation with different GC columns, Bidleman 1984)
- 0.303 (supercooled liquid P_{ L }, converted from literature P_{ S } with \( \Delta S_{ fus } \), Bidleman 1984)
- 0.00332 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
- 0.00205* (41.05°C, gas saturation-GC, measured range 41–100°C, Rordorf 1985)
- \( \log(P/Pa) = 12.3243 - 4336.95/(T/K) - 41.1905 \); temp range 41–100°C (gas saturation, Rordorf 1985)
- 0.00147, 0.187 (20°C, quoted: solid P_{ S }, supercooled liquid P_{ L }, Bidleman & Foreman 1987)
- \( \log(P/kPa) = 7.0076 - 2831.85/(–28.25 + T/K) \); temp range 387–502 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
- \( \log(P/kPa) = 7.35248 - 2786.78/(–61.33 + T/K) \); temp range 502–589 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
- 0.245 (supercooled liquid P_{ L }, Suntio et al. 1988b)
- 0.303, 0.127 (supercooled P_{ L }, converted from literature P_{ S } with different \( \Delta S_{ fus } \) values, Hinckley et al. 1990)
- 0.159, 0.119 (P_{ gc } by GC-RT correlation with different reference standards, Hinckley et al. 1990)
- \( \log(P_{ S }/Pa) = 11.11 - 3582/(T/K) \); temp range –15 to 40°C, Dickhut et al. 1994)
- \( \log(P_{ S }/Pa) = \frac{10.83 - 4044/(T/K)}{20°C} \); temp range –30 to 40°C (derived from gas saturation data, Wania et al. 1994)
- 0.367; 0.344 (supercooled liquid P_{ L }, GC-Kovás retention indices correlation; quoted lit., Speikema et al. 1994)
- \( \log(P/mmHg) = -134.3625 - 1.5459 \times 10^3/(T/K) + 11.748 \log(T/K) - 6.5123 \times 10^{-2}/(T/K) + 2.0872 \times 10^{-5}/(T/K)^2 \); temp range 502–825 K (Yaws 1994)
- 0.0359; 1.46 \times 10^{-3}, 0.141 (liquid P_{ S } from GC-RT correlation; quoted solid P_{ S }, converted to P_{ L }, Donovan 1996)
- (4.6–26) \times 10^{-4}, (1.11–5.40) \times 10^{-3} (quoted exptl. solid P_{ S } ranges: 20°C, Delle Site 1997)
- 0.271; 0.00821 (P_{ L } supercooled liquid, GC-RT correlation; solid P_{ S }, Passivirta et al. 1999)
- \( \log(P_{ S }/Pa) = 8.42 - 2834/(T/K) \); temp range –30 to 40°C (supercooled liquid, Passivirta et al. 1999)
- 0.14, 0.094 (supercooled liquid P_{ L }; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
- \( \log(P_{ S }/Pa) = -3.530/(T/K) + 10.97 \); temp range 14.8–50.5°C, ten Hulscher et al. 1992)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 15.3 (gas stripping-GC, Atlas et al. 1982)
- 48.6 (gas stripping-GC, Oliver 1985)
- 172 (gas stripping-GC, Warner et al. 1987)
- 41756 (computer value, Yaws et al. 1991)
- 41.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

© 2006 by Taylor & Francis Group, LLC
ln \([H/(Pa \, m^3/mol)] = 22.7994 - 5630.6/(T/K)\), temp range 14–50°C (gas stripping-GC, ten Hulscher et al. 1992)

26243, 29587 (26.0, 46.0°C, EPICS-GC, Hansen et al. 1993)

\[\log[H/(Pa \, m^3/mol)] = 7.97 - 1622/(T/K)\] (Passivirta et al. 1999)

35.1 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

\[\log K_{AW} = 6.266 - 2377/(T/K)\] (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

52, 65 (LDV literature-derived value, FA V final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, \(\log K_{ow}\) or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

6.18 (Neely et al. 1974)

4.13 (radioisotope tracer-\(^{14}\)C, Lu & Metcalf 1975)

6.51 (calculated-fragment constant, Rekker 1977)

4.13 (Hansch & Leo 1979)

5.0, 6.27 (shake flask-GC, HPLC-k’ correlation, Könemann et al. 1979)

5.23 (HPLC-RT correlation, Veith et al. 1979b)

6.18 (HPLC-RT correlation, Veith et al. 1979a)

5.44 (shake flask-GC, Briggs 1981)

6.22 (HPLC-RT correlation, McDuffie 1981)

5.56, 5.04–5.92 (shake flask method: mean, range of mean values, OECD 1981)

5.50 (shake flask-GC, Chiu et al. 1982; Chiu 1985)

5.66 (HPLC-RT correlation, Hammers et al. 1982)

5.40 (shake flask-GC, Watarai et al. 1982)

6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)

6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)

5.46, 5.26; 5.47 (Review of HPLC methods; OECD/ECC shake-flask method, Harnisch et al. 1983)

5.47 (generator column-GC/ECD, Miller et al. 1984; 1985)

5.70–5.79 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)

5.75, 5.60, 5.90 (selected OECD value; HPLC-RV correlation, Brooke et al. 1986)

6.92 (HPLC-k’ correlation, De Kock & Lord 1987)

5.64 (HPLC-k’ correlation, Mailhot 1987)

6.22 (HPLC-RT correlation, Doucette & Andren 1988)

5.7* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

5.50 (shake flask-GC, Pereira et al. 1988)

5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)

5.44 (recommended, Sangster 1993)

5.73 (recommended, Hansch et al. 1995)

5.46* ± 0.02 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)

\[\log K_{ow} = 1.1806 - 24.4/[2.303R(T/K)];\] temp range 5–45°C (van’t Hoff eq., Bahadur et al. 1997)

5.845 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

5.55 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

5.52, 5.64 (LDV literature-derived value, FA V final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, \(\log K_{oa}\) at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

6.90*; 6.78 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)

\[\log K_{oa} = -6.30 + 3928/(T/K);\] temp range –10 to 20°C, \(\Delta H_{oa} = 75.2 \, kJ/mol\) (Harner & Mackay 1995)

6.80 (calculated-K_{ow}/K_{aw}, Wania & Mackay 1996)

7.17, 6.90 (calculated-S_{oa} and vapor pressure P, quoted lit., Abraham et al. 2001)


7.38, 7.21 (LDV literature derived value, FA V final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, \(\log BCF\) at 25°C or as indicated:

3.89 (rainbow trout, calculated-rate constant ratio \(k_1/k_2\), Neely et al. 1974)

3.09 (fish, Körte et al. 1978)
4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979b)
5.46 (guppy, lipid basis, Könemann & van Leeuwen 1980;)
4.27 (fish, Ciam et al. 1980)
1.20 (rats, adipose tissue, Geyer et al. 1980)
3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
3.38–4.08 mean 4.08; 3.88–4.30 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
5.16–5.37 (15°C, rainbow trout, lipid basis, Oliver & Niimi 1983; quoted, Chiou 1985)
4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
4.34 (sunfish; rainbow trout, 15°C, Davis & Dobbs 1984)
4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
5.09 (green algae, dry wt basis, Geyer et al. 1985)
4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
2.62–2.97; 2.44–2.79 (human fat: lipid basis, wet weight, Geyer et al. 1987)
4.41 (algae, Mailhot 1987)
4.34 (fathead minnow, Carlson & Kosian 1987)
4.38, 4.30 (worms, fish, Oliver 1987a)
3.48 (fish-normalized, Tadokoro & Tomita 1987)
5.57, 5.62, 5.66, 5.76 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
–1.35, –2.07, –0.32 (beef, milk, vegetable, reported as biotransfer factor log Bb, Travis & Arns 1988)
5.46 (guppy-lipid base, 12 to 31-d exposure studies, Gobas et al. 1989)
3.53 (picea omorika, Reischl et al. 1989)
3.57 (fish, calculated, Figueuroa & Simmons 1991)
4.73; 4.76 (Scenedesmus spp. Coenobia, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
3.74–4.30; 4.21; 4.34; 4.16; (Oncorhynchus mykiss; Poecilia reticulata; Lepomis cyanellus; Oryzias latipes, quoted lit., flow through conditions, Devillers et al. 1996)
5.62 (Poecilia reticulata, quoted lit., static and semi-static conditions, Devillers et al. 1996)
3.18, 4.39 (macrophytes Myriophyllum spicatum, alage Chlorella fusca, wet wt basis, Wang et al. 1996)
5.55 (pond snail Lymnaea stagnalis, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
4.38, 5.08 (algae Chlorella: wet wt basis, dry wt basis, Geyer et al. 2000)
3.98, 5.98 (Daphnia: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 3.54, > 5.54 (mussel Mytilus edulis 21-d non-steady state: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.69, 5.71 (golden orfe Leuciscus idus melanotus, 0.95% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
2.65, 2.83 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.74; 3.95 (Oncorhynchus mykiss, wet wt. basis: quoted expl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K OC:

3.59 (Kenaga & Goring 1980; Kenaga 1980a)
4.45 (Kenaga 1980a)
4.49 (soil, sorption isotherm, converted from reported log KOM of 4.25, Briggs 1981)
2.56 (Speyer soil < 2.00 mm, Freundlich isotherm, Rippen et al. 1982)
2.70 (Alfisol, Freundlich isotherm, Rippen et al. 1982)
5.90; 5.50 (field data of Lake Ontario sediment trap material; Niagara River organic matter, Oliver & Charlton 1984)
4.90, 5.2–6.0 (bottom sediment, range, Karickhoff & Morris 1985)
5.2–6.7, 6.1; 5.80 (suspended sediment, average; algae > 50 µm, Oliver 1987c)
6.0–6.50, 6.30; 5.10 (Niagara River plume: range, mean; calculated-K OW, Oliver 1987b)
4.77 (HPLC-k' correlation, Hodson & Williams 1988)
4.66, 3.08, 4.91 (soil/water, soil-dextran/water, humic acid/water, batch equilibrium-sorption isotherm, Enfield et al. 1989)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

3.23, 4.73; 4.59 (Captina silt loam OC 1.49%, McLaurie sandy loam OC 0.66%; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

5.51 (organic matter, Koelmans et al. 1993)

4.89 ± 0.36; 4.59 (suspended particulates in coastal waters, Masunaga et al. 1996)

4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

4.23, 3.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

5.53, 5.48 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K<sub>OM</sub>:

4.25 (soil-organic matter, sorption isotherm, shake flask-GC, Briggs 1981)

5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization/Evaporation: k = 3.45 × 10<sup>–10</sup> mol m<sup>–2</sup> h<sup>–1</sup> (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, k = 1.44 × 10<sup>–2</sup> h<sup>–1</sup> (Brown et al. 1975; quoted, Mackay et al. 1985); photooxidation k = 3753–37530 h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on k<sub>OH</sub> = 0 was observed after 13 d at pH 3, 7, 11, and 85°C (Ellington et al. 1987, 1988).

Biodegradation: t<sub>1/2</sub>(aq. aerobic) = 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991);

t<sub>1/2</sub>(aq. anaerobic) = 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974; Howard et al. 1991);

degradation rate constant k = 1.9 × 10<sup>–5</sup> h<sup>–1</sup> in soil (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991);

not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982)

t<sub>1/2</sub>(aerobic) = 970 d, t<sub>1/2</sub>(anaerobic) = 3900 d in natural waters (Capel & Larson 1995)

dechlorination pseudo-first order rate constant k = 0.282 d<sup>–1</sup> with t<sub>1/2</sub> = 2.5 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Bioconcentration Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:

k<sub>1</sub> = 18.76 h<sup>–1</sup>; k<sub>2</sub> = 0.00238 h<sup>–1</sup> (trout muscle, Neely et al. 1974)

k<sub>1</sub> = 10000 d<sup>–1</sup> (guppy, Königmann & van Leeuwen 1980)

k<sub>1</sub> = 22.5 h<sup>–1</sup> (guppy, quoted from Königmann & van Leeuwen 1980, Hawker & Connell 1985)

log k<sub>1</sub> = 1.35 d<sup>–1</sup> (fish, quoted from Königmann & van Leeuwen 1980, Hawker & Connell 1985)

k<sub>1</sub> = 18.8 h<sup>–1</sup> (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

log k<sub>1</sub> = 1.27 d<sup>–1</sup> (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

1/k<sub>2</sub> = 420 h (trout, quoted from Bruggeman et al. 1984, Hawker & Connell 1985)

log k<sub>2</sub> = 2.62 d<sup>–1</sup> (fish, quoted, Hawker & Connell 1985)

k<sub>2</sub> = 540 d<sup>–1</sup> (fish, quoted, Oppenhuizen 1986)

k<sub>1</sub> = 0.00510, 0.00818, 0.00640, 0.0047 d<sup>–1</sup> (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)

log k<sub>1</sub> = 2.73 d<sup>–1</sup> (fish, quoted from Königmann & van Leeuwen 1980, Connell & Hawker 1988)

log k<sub>1</sub> = 2.65 d<sup>–1</sup>; log 1/k<sub>2</sub> = 1.24 d (fish, quoted from Bruggeman et al. 1984, Connell & Hawker 1988)

log k<sub>2</sub> = –1.24 d<sup>–1</sup> (fish, calculated-K<sub>OW</sub>, Thomann 1989)

k<sub>1</sub> = 0.049 h<sup>–1</sup>; k<sub>2</sub> = 0.023 h<sup>–1</sup> (mayfly-sediment model II, Gobas et al. 1998)

k<sub>1</sub> = 0.092 d<sup>–1</sup> with elimination t<sub>1/2</sub> = 7.5 d (earthworm, Belfroid et al. 1995)

k<sub>1</sub> = 6.558 h<sup>–1</sup>, k<sub>2</sub> = 0.00429 h<sup>–1</sup> (Macrophytes Myriophyllum spicatum, Wang et al. 1996)

k<sub>1</sub> = 10489 h<sup>–1</sup>, k<sub>2</sub> = 0.424 h<sup>–1</sup> (algae Chlorella fusca, Wang et al. 1996)

k<sub>1</sub> = 0.016 d<sup>–1</sup> with t<sub>1/2</sub> = 43 d and k<sub>2</sub> = 0.017 d<sup>–1</sup> with t<sub>1/2</sub> = 42 d for food concn of 14 ng/g and 103 ng/g respectively in a 30-d uptake followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k<sub>1</sub> = 467 mL g<sup>–1</sup> d<sup>–1</sup>, k<sub>2</sub> = 0.26 d<sup>–1</sup> (pond snail Lymnaea stagnalis, Legierse et al. 1998)

k<sub>1</sub> = 8 (food lipid mg)/(g worm lipid-d) (earthworm, Wågman et al. 2001)
Half-Lives in the Environment:

Air: \( t_{1/2} = 3753–37530 \) h, based on estimated photooxidation half-life (Atkinson 1987, Howard et al. 1991)
\( t_{1/2} = 29 \pm 5.8 \) yr at Eagle Harbor, \( t_{1/2} = 15 \pm 1.9 \) yr at Sleeping Bear Dunes and \( t_{1/2} = 18 \pm 2.3 \) yr in the Great Lakes = atmosphere at Sturgeon Point (Buehler et al. 2004).

Surface Water: \( t_{1/2} = 1.4–50 \) d estimated, \( t_{1/2} = 0.3–3 \) d for river water and \( t_{1/2} = 30–300 \) d for lakes, estimated from persistence (Zoeteman et al. 1980)
\( t_{1/2} = 23256–50136 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)
\( t_{1/2}(\text{aerobic}) = 970 \) d, \( t_{1/2}(\text{anaerobic}) = 3900 \) d in natural waters (Capel & Larson 1995)

Groundwater: \( t_{1/2} = 30–300 \) d, estimated from persistence (Zoeteman et al. 1980)
\( t_{1/2} = 46512–100272 \) h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)

Sediment: dechlorination \( t_{1/2} = 1.8 \) d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil: \( t_{1/2} > 50 \) d (Ryan et al. 1988)
disappearance \( t_{1/2} = 11.3 \) d from testing soils (Anderson et al. 1991)
\( t_{1/2} = 23256–50136 \) h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991)
\( t_{1/2} = 3–6 \) yr in soil (Geyer et al. 2000)
\( t_{1/2} = 48.7 \) and 11.7 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: \( t_{1/2} = 163 \) h, clearance from fish (Neely 1980)
\( t_{1/2} > 224 \) d in rainbow trout (Niimi & Cho 1980);
\( t_{1/2} = 210 \) d at 4°C, \( t_{1/2} = 80 \) d at 12°C, \( t_{1/2} = 70 \) d at 18°C in subadult rainbow trout (Niimi & Palazzo 1985)
\( t_{1/2} = 27 \) d in worms at 8°C (Oliver 1987a)
biological \( t_{1/2} = 12 \) d in trout muscle, \( t_{1/2} > 173 \) d and > 224 d in trout, \( t_{1/2} = 12 \) d in guppy (Niimi 1987);
\( t_{1/2} = 30 \) d in \textit{picea omorika} (Reischl et al. 1989)
elimination \( t_{1/2} = 1.44 \) d and 12.3 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994)
elimination \( t_{1/2} = 1.9–7.5 \) d from earthworm in soil (Belfroid et al. 1995)
Depuration \( t_{1/2} = 42–43 \) d in a 30-d dietary exposure and 160-d duputation studies (juvenile rainbow trout, Fisk et al. 1998)

### TABLE 6.1.1.12.1

Reported aqueous solubilities and Henry’s law constants of hexachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Solubility</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>gen. col./elution method</td>
<td>generator column-GC/ECD</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
</tr>
<tr>
<td>15</td>
<td>0.00921(^{1})</td>
</tr>
<tr>
<td>25</td>
<td>0.00996(^{2})</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{mean, 0.00206–0.0216 g/m}^3 )</td>
<td>35</td>
</tr>
<tr>
<td>( \text{mean, 0.00119–0.0231 g/m}^3 )</td>
<td>45</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( \Delta H_{\text{sol}} = 33.7 \text{ kJ/mol} \)

\( \Delta H_{\text{sol}} = 33.5 \text{ kJ/mol} \)
FIGURE 6.1.1.12.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.2
Reported vapor pressures of hexachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[ \log P = A - \frac{B}{T/K} \] (1)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = A - \frac{B}{C + t/°C} \] (2)
\[ \log \left( \frac{P}{\text{Pa}} \right) = A - \frac{B}{C + T/K} \] (3)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>summary lit. data</td>
<td>Rodebush gauge</td>
<td>gas saturation-GC</td>
<td>gas saturation/balance</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>measured 96–124°C</td>
<td>P/mmHg</td>
<td>P/Pa</td>
</tr>
<tr>
<td>114.1</td>
<td>133</td>
<td></td>
<td>15</td>
<td>0.000528</td>
</tr>
<tr>
<td>149.3</td>
<td>667</td>
<td></td>
<td>25</td>
<td>0.00255</td>
</tr>
<tr>
<td>166.4</td>
<td>1333</td>
<td>eq. 1 P/mmHg</td>
<td>35</td>
<td>0.00853</td>
</tr>
<tr>
<td>185.7</td>
<td>2666</td>
<td>A</td>
<td>45</td>
<td>0.0279</td>
</tr>
<tr>
<td>206</td>
<td>5333</td>
<td>B</td>
<td>25</td>
<td>0.0023</td>
</tr>
<tr>
<td>219</td>
<td>7999</td>
<td></td>
<td></td>
<td>50</td>
</tr>
<tr>
<td>235.5</td>
<td>13332</td>
<td></td>
<td>10</td>
<td>0.00028</td>
</tr>
<tr>
<td>258.8</td>
<td>26664</td>
<td></td>
<td>20</td>
<td>0.0011</td>
</tr>
<tr>
<td>283.5</td>
<td>53329</td>
<td></td>
<td>30</td>
<td>0.003</td>
</tr>
<tr>
<td>309.4</td>
<td>101325</td>
<td></td>
<td>40</td>
<td>0.013</td>
</tr>
<tr>
<td>mp/°C</td>
<td>230</td>
<td></td>
<td>50</td>
<td>0.039</td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>t/°C</td>
</tr>
<tr>
<td></td>
<td>gas saturation</td>
<td>gas saturation-GC</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>41.05</td>
<td>0.0205</td>
<td>-15</td>
<td>-30</td>
</tr>
<tr>
<td>50.16</td>
<td>0.0547</td>
<td>-5.0</td>
<td>-20</td>
</tr>
<tr>
<td>60.3</td>
<td>0.165</td>
<td>10</td>
<td>-10</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>Rordorf 1985</th>
<th>Liu &amp; Dickhut 1994</th>
<th>Wania et al. 1994</th>
</tr>
</thead>
<tbody>
<tr>
<td>70.3</td>
<td>0.452</td>
<td>25</td>
<td>3.11 × 10⁻³</td>
<td>0</td>
</tr>
<tr>
<td>80.3</td>
<td>1.155</td>
<td>40</td>
<td>0.121</td>
<td>1.03 × 10⁻⁴</td>
</tr>
<tr>
<td>90.4</td>
<td>2.77</td>
<td>20</td>
<td>1.092 × 10⁻³</td>
<td>3.556 × 10⁻⁴</td>
</tr>
<tr>
<td>100.25</td>
<td>6.29</td>
<td>∆H_v/(kJ mol⁻¹) = 81.3</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>101.25</td>
<td>6.29</td>
<td>P/Pa</td>
<td>eq. 1</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>12.3243</td>
<td>∆H_mel/(kJ mol⁻¹) = 105</td>
<td>A</td>
<td>10.83</td>
</tr>
<tr>
<td>B</td>
<td>4336.95</td>
<td>B</td>
<td>4044</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-41.1905</td>
<td>∆H_v/(kJ mol⁻¹) =: 77.4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Hexachlorobenzene: vapor pressure vs. 1/T

**FIGURE 6.1.12.2** Logarithm of vapor pressure versus reciprocal temperature for hexachlorobenzene.
### TABLE 6.1.1.12.3
Reported octanol-water partition coefficients and octanol-air partition coefficients of hexachlorobenzene at various temperatures

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-GC/ECD</td>
<td>shake flask-GC/ECD</td>
<td>generator column-GC</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>T/°C</td>
<td>log K_{OW}</td>
<td>T/°C</td>
<td>log K_{OW}</td>
<td>T/°C</td>
</tr>
<tr>
<td>13</td>
<td>5.68</td>
<td>5</td>
<td>5.74</td>
<td>25</td>
</tr>
<tr>
<td>19</td>
<td>5.7</td>
<td>15</td>
<td>5.6</td>
<td>–10</td>
</tr>
<tr>
<td>28</td>
<td>5.58</td>
<td>25</td>
<td>5.46</td>
<td>0</td>
</tr>
<tr>
<td>33</td>
<td>4.66</td>
<td>35</td>
<td>5.3</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
<td>5.17</td>
<td>18.5</td>
</tr>
</tbody>
</table>

\(\Delta H/(kJ \text{ mol}^{-1}) = -24.4\) enthalpy of transfer

\(\Delta H/(kJ \text{ mol}^{-1}) = -24.4\)

\(\log K_{OW} = A - \Delta H/2.303RT\)

A 1.1806

\(\log K_{OA} = A + B/T\)

A –6.3

\(\Delta H = -24400\)

B 3928

\(\Delta \text{HOA/(kJ mol}^{-1}) = 75.2\)

\(\Delta \text{HOA/(kJ mol}^{-1}) = 55.8\)

\(\log K_{OW} = A - \Delta H/2.303RT\)

A 1.1806

\(\log K_{OA} = A + B/T\)

A –2.395

\(\Delta H = -24400\)

B 3928

\(\Delta \text{HOA/(kJ mol}^{-1}) = 75.2\)

\(\Delta \text{HOA/(kJ mol}^{-1}) = 55.8\)

**FIGURE 6.1.1.12.3** Logarithm of \(K_{OW}\) and \(K_{OA}\) versus reciprocal temperature for hexachlorobenzene.
6.1.2 CHLOROTOLUENES

6.1.2.1 2-Chlorotoluene

- Common Name: 2-Chlorotoluene
- Synonym: o-Tolylechloride, o-chlorotoluene, 2-chloro-1-methylbenzene
- Chemical Name: 2-chlorotoluene
- CAS Registry No: 95-49-8
- Molecular Formula: C7H7Cl
- Molecular Weight: 126.584
- Melting Point (°C): –35.8 (Lide 2003)
- Boiling Point (°C):
  - 159.15 (Dreisbach 1955; Weast 1982–83)
  - 159.0 (Dean 1985, 1992)
- Density (g/cm³ at 20°C):
  - 1.08245, 1.07762 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
- Molar Volume (cm³/mol):
  - 116.9 (20°C, calculated-density)
  - 139.1 (calculated-Le Bas method at normal boiling point)
- Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol): 8.368 (Dreisbach 1955; Riddick et al. 1986)
- Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
  - Fugacity Ratio at 25°C, F: 1.0
- Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
  - 372 (Isnard & Lambert 1989)
  - 252.0 (shake flask, Fredenlund et al. 1995)
  - 117* ± 5.1 (shake flask-GC/FID, Ma et al. 2001)
- Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  - 487 (interpolated-Antoine eq., Stuckey & Saylor 1940)
  - $\log P/mmHg = 7.29547 – 1701.60/(T/K – 45.42)$; temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
  - 133.3*, 666.6, 1333 (5.4, 30.6, 43.2°C, summary of lit. data, temp range 5.4–159°C, Stull 1947)
  - 482.5 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986, Howard 1993)
  - $\log (P/mmHg) = 6.94763 – 1497.2/(209.0 + t°C)$; temp range 65–220°C (Antoine eq., Weast 1972–73)
  - 485 (interpolated-Antoine eq., Dean 1985, 1992)
  - $\log (P/mmHg) = 7.36797 – 1735.8/(t°C + 230.0)$; temp range 0–65°C (Antoine eq., Dean 1985, 1992)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

\[ \log \left( \frac{P}{P_0} \right) = 6.07253 - 1497.2/(T/\text{K} - 64.15); \text{ temp range 338–493K (liquid, Antoine eq., Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{mmHg}) = 33.2792 - 3.4099 \times 10^3/(T/\text{K}) - 8.6743 \times 10^{-6}(T/\text{K}) + 6.8174 \times 10^{-10}(T/\text{K})^2, \text{ temp range 237–656 K (Yaws 1994)} \]

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):


\[ \ln (k_H/\text{atm}) = 17.18 - 3545/(T/\text{K}); \text{ temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)} \]

295 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

\[ \log K_{AW} = 3.890 - 1409/(T/\text{K}) \text{ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)} \]

Octanol/Water Partition Coefficient, log \( K_{OW} \):

3.42 (shake flask, Leo et al. 1971, Hansch & Leo 1979, Hansch et al. 1995)

3.52 (HPLC-RT correlation, Könemann et al. 1979)

3.40 (HPLC-\( k' \) correlation, Hanai et al. 1981)

3.59 (RP-HPLC-RT correlation, Edsforth 1986)

3.52 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 6.1.2.1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities, vapor pressures and Henry’s law constants of 2-chlorotoluene at various temperatures</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-GC</td>
<td>summary of lit. data</td>
<td>equilibrium cell-GC</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/g\cdot m^{-3} )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>5</td>
<td>89.4</td>
<td>5.4</td>
</tr>
<tr>
<td>15</td>
<td>97.1</td>
<td>30.6</td>
</tr>
<tr>
<td>25</td>
<td>117</td>
<td>43.2</td>
</tr>
<tr>
<td>35</td>
<td>128</td>
<td>56</td>
</tr>
<tr>
<td>45</td>
<td>132</td>
<td>72</td>
</tr>
<tr>
<td>81.8</td>
<td></td>
<td>81.8</td>
</tr>
<tr>
<td>115</td>
<td>26664</td>
<td>115.995</td>
</tr>
<tr>
<td>137.1</td>
<td>53329</td>
<td>121.252</td>
</tr>
<tr>
<td>159</td>
<td>101325</td>
<td>126.313</td>
</tr>
<tr>
<td></td>
<td></td>
<td>139.532</td>
</tr>
<tr>
<td></td>
<td></td>
<td>147.287</td>
</tr>
<tr>
<td></td>
<td></td>
<td>155.689</td>
</tr>
<tr>
<td></td>
<td></td>
<td>158.323</td>
</tr>
<tr>
<td></td>
<td>158.849</td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 6.1.2.1.1 Logarithm of mole fraction solubility, vapor pressure and Henry’s law constant versus reciprocal temperature for 2-chlorotoluene.
6.1.2.2 3-Chlorotoluene

Common Name: 3-Chlorotoluene
Synonym: m-Tolylchloride, 3-chloro-1-methylbenzene
Chemical Name: 3-chlorotoluene
CAS Registry No: 108-41-8
Molecular Formula: C\textsubscript{7}H\textsubscript{7}Cl
Molecular Weight: 126.584

Melting Point (°C):
-47.8 \, (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):
161.8 \, (Dean 1985; 1992; Lide 2003)

Density (g/cm\textsuperscript{3} at 20°C):
1.0722 \, (Weast 1982–83)
1.0728 \, (20°C, Riddick et al. 1986)

Molar Volume (cm\textsuperscript{3}/mol):
118.1 \, (20°C, calculated-density, Stephenson & Malanowski 1987)
139.1 \, (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 43.76 \, (Riddick et al. 1986)

Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):

Fugacity Ratio at 25°C, \(F\): 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
372 \, (Isnard & Lambert 1989)
117* ± 2.1 \, (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
418 \, (interpolated-Antoine eq., Stuckey & Saylor 1940)
\log P/mmHg = 7.62515 – 1887.31/(T/K – 33.40); temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
133.3*, 666.6, 1333 (4.8, 30.3, 43.2°C, summary of lit. data, temp range 4.8–162.3°C, Stull 1947)
488.9 \, (extrapolated, Antoine eq., Weast 1972–73)
\log (P/kPa) = -(0.2185 \times 10081.1)/(T/K) + 7.952234; temp range 4.8–162.3°C (Antoine eq., Weast 1982–83)
403.0 \, (extrapolated-Antoine eq., Boublik et al. 1984)
\log (P/kPa) = 6.09068 – 1511.858/(t/°C + 208.119); temp range 64.8–159.8°C (Antoine eq., Boublik et al. 1984)
670.0 \, (Riddick et al. 1986)
\log (P/kPa) = 6.2794 – 1637.6/(223.3 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
512.2 \, (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\log (P/kPa) = 6.93017 – 2028.13/(T/K) – 11.629]; temp range 277–436 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):

Octanol/Water Partition Coefficient, log \(K_{ow}\):
3.28 \, (shake flask, Leo et al. 1971, Hansch & Leo 1979)
3.40 \, (HPLC-k’ correlation, Hanai et al. 1981)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:

### TABLE 6.1.2.2.1
Reported aqueous solubilities and vapor pressures of 3-chlorotoluene at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ma et al. 2001</strong></td>
<td><strong>Stull 1947</strong></td>
</tr>
<tr>
<td><strong>shake flask-GC</strong></td>
<td><strong>summary of literature data</strong></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>101</td>
</tr>
<tr>
<td>15</td>
<td>99.3</td>
</tr>
<tr>
<td>25</td>
<td>117</td>
</tr>
<tr>
<td>35</td>
<td>113</td>
</tr>
<tr>
<td>45</td>
<td>128</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$mp/°C$</td>
</tr>
</tbody>
</table>

**FIGURE 6.1.2.2.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 3-chlorotoluene.
6.1.2.3 4-Chlorotoluene

Common Name: 4-Chlorotoluene
Synonym: p-Tolylchloride, 4-chloro-1-methylbenzene
Chemical Name: 4-chlorotoluene
CAS Registry No: 106-43-4
Molecular Formula: C7H7Cl
Molecular Weight: 126.584
Melting Point (°C):
  7.5  (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  162.4  (Lide 2003)
Density (g/cm³ at 20°C):
  1.0697  (Weast 1982–83; Riddick et al. 1986; Dean 1985, 1992; Lide 2003)
Molar Volume (cm³/mol):
  118.3  (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
  139.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
  106.0  (20°C, Yalkowsky 1987)
  123* ± 6.1  (shake flask-GC/FID, Ma et al. 2001)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  422  (interpolated-Antoine eq., Stuckey & Saylor 1940)
  log P/mmHg = 23.07210 – 3041.02/(T/K) – 5·log (T/K); temp range 4–75°C (vapor pressure eq. based on expctl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)
  133.3*, 666.6, 1333 (5.5, 31.0, 43.8°C, temp range 5.5–162.3°C, summary of lit. data, Stull 1947)
  471.6  (interpolated, Antoine eq., Weast 1982–83)
  log (P/mmHg) = (–0.2185 × 10151.7)/(T/K) + 7.988366); temp range 5.5–162.3°C (Antoine eq., Weast 1982–83)
  log (P/mmHg) = 6.09068 – 1511.858/(t/°C + 208.199); temp range 65–160°C (Antoine eq., Boublík et al. 1984)
  670  (30.3°C, Riddick et al. 1986)
  log (P/kPa) = 6.75005 – 1887.31/(239.75 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
  506.7  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  log (P/kPa) = 6.90317 – 2107.52/(T/K – 5.373); temp range 304–436 K (Antoine eq., Stephenson & Malanowski 1987)
  log (P/mmHg) = 61.8901 – 4.3760 × 10¹/(T/K) – 19.840·log (T/K) + 7.991 × 10⁻³·(T/K) + 1.0781 × 10⁻¹³·(T/K)², temp range 281–660 K (Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
  412.4  (calculated-P/C, Howard 1993)
Octanol/Water Partition Coefficient, log K_{OW}:

3.33  (shake flask, Leo et al. 1971; Hansch & Leo 1979; 1985)
3.42  (HPLC-RT correlation, Könemann et al. 1979)
3.40  (HPLC-k' correlation, Hanai et al. 1981)
3.30  (shake flask, Wang et al. 1987)
3.33  (recommended, Sangster 1993)
3.33  (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.65–2.30  (estimated from log K_{OW}, Lyman et al. 1990; Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

2.65–3.19  (estimated from log K_{OW}, Lyman et al. 1990; Howard 1993)
4.10  (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k or Half-Lives, t\textsubscript{1/2}:

Volatileization: based on the Henry’s law constant, the volatilization t\textsubscript{1/2} \approx 3.5 h from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k\textsubscript{1}) and Elimination (k\textsubscript{2}) Rate Constants:

Half-Lives in the Environment:

Air: t\textsubscript{1/2} = 8.4 d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Atkinson 1987; quoted, Howard 1993).

Surface water: t\textsubscript{1/2} = 1.2 d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)
### TABLE 6.1.2.3.1
Reported aqueous solubilities and vapor pressures of 4-chlorotoluene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>5</th>
<th>Ma et al. 2001</th>
<th>99</th>
<th>shake flask-GC</th>
<th>5.50</th>
<th>Stull 1947</th>
<th>64.855</th>
<th>3584</th>
<th>Cervenkova &amp; Boublik 1982</th>
<th>64.855</th>
<th>3584</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>103</td>
<td></td>
<td></td>
<td></td>
<td>31.0</td>
<td>666.6</td>
<td>75.304</td>
<td>5727</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>123</td>
<td></td>
<td></td>
<td></td>
<td>43.8</td>
<td>1333</td>
<td>84.258</td>
<td>8333</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>136</td>
<td></td>
<td></td>
<td></td>
<td>57.8</td>
<td>2666</td>
<td>91.408</td>
<td>11078</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>153</td>
<td></td>
<td></td>
<td></td>
<td>73.5</td>
<td>5333</td>
<td>97.416</td>
<td>13924</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>83.2</td>
<td>7999</td>
<td>102.574</td>
<td>16819</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>96.6</td>
<td>13332</td>
<td>107.91</td>
<td>20322</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>117.1</td>
<td>26664</td>
<td>113.464</td>
<td>24580</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>139.8</td>
<td>53329</td>
<td>118.857</td>
<td>29380</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>162.3</td>
<td>101325</td>
<td>124.14</td>
<td>34794</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>129.212</td>
<td>40761</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>134.395</td>
<td>47661</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>142.507</td>
<td>60218</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>150.285</td>
<td>74704</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>158.718</td>
<td>93384</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>159.801</td>
<td>96011</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>162.4 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>161.904</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.2.3.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 4-chlorotoluene.
6.1.2.4 2,4-Dichlorotoluene

Common Name: 2, 4-Dichlorotoluene
Synonym: 2, 4-dichloro-1-methylbenzene
Chemical Name: 2, 4-dichlorotoluene
CAS Registry No: 95-73-8
Molecular Formula: C_{7}H_{6}Cl_{2}
Molecular Weight: 161.029

Melting Point (°C):

Boiling Point (°C):
201 (Lide 2003)

Density (g/cm³ at 20°C):
1.2498 (Weast 1982–83)
1.2476 (Riddick et al. 1986, Lide 2003)
1.246 (Dean 1985, 1992)

Molar Volume (cm³/mol):
128.6 (calculated-density, Stephenson & Malanowski 1987)
160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
26.20 ± 2.1 (shake flask-GC/FID, Ma et al. 2001)
18.9, 26.2, 30.7, 37 (15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)
25.9 ± 2.2 (generator column-GC/FID, Ma et al. 2001)
22.3, 23.1, 25.9, 32, 36.6 (5, 15, 25, 35, 45°C, generator column-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
55.5 (Riddick et al. 1986)
log (P/kPa) = 5.6199 – 1330.4/(t/°C + 168.5) (Antoine eq., Riddick et al. 1986)
55.51 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.6199 –1330.4/(T/K – 104.65); temp range 346–475 K (Antoine eq., Stephenson & Malanowski 1987)
61.06 (Daubert & Danner 1989)
log (P/mmHg) = 31.9325 – 3.7438 × 10³/(T/K) – 8.0123-log (T/K) – 7.5077 × 10⁻¹¹(T/K) + 1.250 × 10⁻⁶(T/K)²,
     temp range 260–705 K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
350.6 (calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{ow}:
4.24 (HPLC-RT correlation, Könemann et al. 1979)
4.24 (recommended, Sangster 1993)
4.24 (shake flask, Hansch et al. 1995)
Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

\[ 2.99 \text{ (estimated from } \log K_{OW}, \text{ Howard 1997) } \]

Sorption Partition Coefficient, \( \log K_{OC} \):

\[ 3.68 \text{ (estimated from } \log K_{OW}, \text{ Howard 1997) } \]

Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

Volatileization: \( t_{1/2} = 4.0 \) h in a model river 1-m deep with a 1 m/s current and a 3 m/s wind, \( t_{1/2} = 1 \) d in the Rhine River in the Netherlands (Howard 1997)

Photolysis:

Oxidation: photooxidation \( t_{1/2} = 11.6 \) d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: \( t_{1/2} = 11.6 \) d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Surface water: \( t_{1/2} = 1.0 \) d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Volatileization \( t_{1/2} = 4 \) h in a model river, \( t_{1/2} = 1 \) d in Rhine River in the Netherlands (Howard 1993)
6.1.2.5 2,6-Dichlorotoluene

\[
\begin{array}{c}
\text{Cl} \\
\text{Cl}
\end{array}
\]

Common Name: 2, 6-Dichlorotoluene  
Synonym:  
Chemical Name: 2, 6-dichlorotoluene  
CAS Registry No: 118-69-4  
Molecular Formula: \(\text{C}_7\text{H}_6\text{Cl}_2\)  
Molecular Weight: 161.029  
Melting Point (°C): liquid  
\[25.8\] (Lide 2003)  
Boiling Point (°C):  
\[198\] (Weast 1982–83, Lide 2003)  
Density (g/cm\(^3\)) at 20°C:  
\[1.254\] (Dean 1992)  
\[1.2686\] (Lide 2003)  
Molar Volume (cm\(^3\)/mol):  
\[126.9\] (20°C, calculated-density)  
\[160.0\] (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):  
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):  
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):  
Fugacity Ratio at 25°C, \(F\): 1.0  
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):  
\[23.3 \pm 0.81\] (shake flask-GC/FID, Ma et al. 2001)  
\[16.7, 19.8, 23.3, 30.1, 33\] (5, 15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)  
Vapor Pressure (Pa at 25°C):  
\[53.19\] (estimated, Lyman et al. 1990, Howard 1997)  
Henry’s Law Constant (Pa-m\(^3\)/mol):  
\[350.6\] (Hine & Mookerjee 1975)  
Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):  
\[4.29\] (HPLC-\(k'\) correlation, Könemann et al. 1979)  
\[4.29\] (recommended, Sangster 1983)  
\[4.29\] (recommended, Hansch et al. 1995)  
Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\):  
Bioconcentration Factor, log BCF:  
\[3.03\] (estimated from log \(K_{\text{OW}}\), Howard 1997)  
Sorption Partition Coefficient, log \(K_{\text{OC}}\):  
\[3.71\] (estimated from log \(K_{\text{OW}}\), Howard 1997)  
Environmental Fate Rate Constants, \(k\) or Half-Lives, \(t_{\frac{1}{2}}\):  
Volatilization: based on Henry’s law constant, an estimated \(t_{\frac{1}{2}} = 4.0\) h of volatilization from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Howard 1997).  
Photolysis:
Oxidation: photooxidation $t_{1/2} = 11.6$ d in the atmosphere for reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 11.6$ d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).
6.1.2.6 3,4-Dichlorotoluene

Common Name: 3, 4-Dichlorotoluene
Synonym: 3, 4-dichloro-1-methylbenzene
Chemical Name:
CAS Registry No: 95-75-0
Molecular Formula: C7H6Cl2
Molecular Weight: 161.029
Melting Point (°C):
Boiling Point (°C):
208.9 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
1.25256, 1.24751 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
1.2564 (Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
127.9 (calculated-density, Stephenson & Malanowski 1987)
160.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
13.33, 10.13 (25°C, bp, Dreisbach 1955; Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
10.544 (Dreisbach 1955)
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
26 (30°C, Dreisbach 1955; IUPAC Solubility Data Series, Horvath & Getzen 1985; Riddick et al. 1986)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
42 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.97925 – 1655.4/(195.0 + t°C); temp range 105–270°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = 6.91048 – 946.35/(246.68 + t°C); temp range -87 to 7°C (Antoine eq., Dean 1985, 1992)
42.0 (Riddick et al. 1986)
log (P/kPa) = 6.10415 – 1655.44/(195.0 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 6.10415 – 1655.44/(T/K – 78.15); temp range 378–543 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log KOW:
4.067 (Verhaar et al. 1992)
Octanol/Air Partition Coefficient, log KOA:
Bioconcentration Factor, log BCF or log KB:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Half-Lives in the Environment:
6.1.2.7 2,3,6-Trichlorotoluene

Common Name: 2, 3, 6-Trichlorotoluene
Synonym:
Chemical Name: 2, 3, 6-trichlorotoluene
CAS Registry No: 2077-46-5
Molecular Formula: C_7H_5Cl_3
Molecular Weight: 195.474
Melting Point (°C):
45–46 (Weast 1982–83)
Boiling Point (°C):
229.5 (Weast 1982–83)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
180.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.629 (mp at 45.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.08 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_v/kPa) = 5.6249 – 1323/(T/K – 144.15); temp range 384–509 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
152 (gas stripping-GC, Oliver 1985)
245 (calculated-bond contribution method, Meylan & Howard 1991)
Octanol/Water Partition Coefficient, log K_{ow}:
4.80 (calculated as per Hansch & Leo 1979, Oliver 1987b)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:
Half-Lives in the Environment:
Biota: elimination t_1/2 < 5 d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b)
6.1.2.8 2,4,5-Trichlorotoluene

Common Name: 2, 4, 5-Trichlorotoluene
Synonym: 2, 4, 5-TCT
Chemical Name: 2, 4, 5-trichlorotoluene
CAS Registry No: 6639-30-1
Molecular Formula: C₇H₅Cl₃
Molecular Weight: 195.474

Melting Point (°C):
82.4  (Weast 1982–83; Lide 2003)

Boiling Point (°C):
231  (Lide 2003)

Density (g/cm³ at 20°C):
1.1004  (Lide 2003)

Molar Volume (cm³/mol):
115.0  (20°C, calculated-density)
180.9  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):

Enthalpy of Fusion, ∆Hₓ (kJ/mol):

Entropy of Fusion, ∆S₃ (J/mol K):

Fugacity Ratio at 25°C (assuming ∆S₃ = 56 J/mol K), F: 0.273 (mp at 82.4°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
2.33 ± 0.22  (shake flask-GC/FID, Ma et al. 2001)
1.10, 1.38, 2.33, 3.33, 5.64 (5, 15, 25, 35, 45°C, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa-m³/mol at 25°C):
152  (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, log Kₗw:
4.82  (calculated-π method of Hansch & Leo 1979, Oliver & Niimi 1984, 1985)
4.80  (Oliver & Niimi 1985)
4.780  (Verhaar et al. 1992)

Bioconcentration Factor, log BCF:
3.68  (rainbow trout, Oliver & Niimi 1984; Oliver 1987)
3.54–3.99 with mean value of 3.88; 3.52–4.04 with mean value of 3.93 (rainbow trout, wet wt., 15°C, steady-state BCF on 7- to 96-d laboratory study on two tanks of different water concn, Oliver & Niimi 1985)

Environmental Fate Rate Constants, k, or Half-Lives, t₁/²;
Half-Lives in the Environment:

Air:
Surface water: $t_{\text{1/2}} = 1.8$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Groundwater:
Sediment:
Soil:
Biota: elimination $t_{\text{1/2}} < 5$ d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b).
6.1.2.9 α-Chlorotoluene

Common Name: α-Chlorotoluene
Synonym: chloromethylbenzene, benzyl chloride
Chemical Name:
CAS Registry No: 100-44-7
Molecular Formula: C₇H₇Cl, C₆H₅CH₂Cl
Molecular Weight: 126.584
Melting Point (°C):
–45 (Lide 2003)
Boiling Point (°C):
179 (Lide 2003)
Density (g/cm³ at 20°C):

Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
493 (20°C, Riddick et al. 1986)
579 (calculated-fragment const., Wakita et al. 1986)
236 (calculated-group contribution, Kühne et al. 1995)
409 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
159.4, 122, 178, 216, 243.5, 320, 322, 370 (1.0, 3.0, 12.4, 12.5, 17.9, 19.1, 22.7, 23.0°C, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
ln (kₜ/atm) = 17.18 – 3545/(T/K); temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
36.07 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

Octanol/Water Partition Coefficient, log $K_{ow}$;
Octanol/Air Partition Coefficient, log $K_{oa}$;
Bioconcentration Factor, log BCF or log $K_{bi}$;
Sorption Partition Coefficient, log $K_{sc}$;

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$, for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3, as indicated, *data at other temperatures see reference:

$k_{O3} < 0.04 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K with a tropospheric lifetimes $\tau > 290$ d and $\tau \sim 3$ d due to reactions with O3 and OH radical at room temp. (Atkinson et al. 1982)

$k_{OH} = (2.95 \pm 0.15) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a atmospheric lifetime $\tau = 3.9$ d at room temp. (relative rate method, Edney et al. 1986)

$k_{OH}(calc) = 2.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs) = 2.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 2.90 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

$t_{1/2} = 22–218$ h, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant $k = 1.28 \times 10^{-5}$ s$^{-1}$ and $t_{1/2} = 15$ h at 25°C and pH 7 (Mabey & Mill 1978)
neutral rate constant $k = 8.5 \pm 0.5$ min$^{-1}$ at 25°C (Ellington et al. 1988)

$t_{1/2} = 25–290$ h based on overall hydrolysis rate constant (Howard et al. 1991)

Biodegradation: $t_{1/2}$(aerobic) = 168–672 h, based on unacclimated aqueous screening test data; $t_{1/2}$(anaerobic) = 672–2688 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetimes $\tau > 290$ d and $\tau \sim 3$ d due to reactions with O3 and OH radical, respectively, at room temp. (Atkinson et al. 1982);
calculated atmospheric lifetime $\tau = 3.9$ d due to reaction with OH radical at room temp. (Edney et al. 1986)

$t_{1/2} = 22–218$ h, based on photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2} = 15–290$ h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Groundwater: $t_{1/2} = 15–290$ h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 15–290$ h, based on estimated hydrolysis half-lives (Howard et al. 1991)

Biota:

---

**TABLE 6.1.2.9.1**

Reported vapor pressures of a-chlorotoluene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$\log P$ = A – B/(T/K)</th>
<th>(1)</th>
<th>$\ln P$ = A – B/(T/K)</th>
<th>(1a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\log (P/mmHg)$ = A – B/(C + t°C)</td>
<td>(2)</td>
<td>$\ln P$ = A – B/(C + t°C)</td>
<td>(2a)</td>
</tr>
<tr>
<td>$\log (P/Pa)$ = A – B/(T/K)</td>
<td>(3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\log (P/mmHg)$ = A – B/(T/K) – C·log (T/K)</td>
<td>(4)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Stull 1947**

<table>
<thead>
<tr>
<th>summary of lit. data</th>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.0</td>
<td>133</td>
<td></td>
</tr>
<tr>
<td>47.8</td>
<td>666.6</td>
<td></td>
</tr>
<tr>
<td>60.8</td>
<td>1333</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>47.8</td>
<td>53.37</td>
</tr>
<tr>
<td>60.8</td>
<td>70.60</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.0</td>
<td>1333</td>
</tr>
<tr>
<td>47.8</td>
<td>666.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>60.8</td>
<td>1333</td>
</tr>
</tbody>
</table>

**Ashcroft 1976**

<table>
<thead>
<tr>
<th>isoteniscope method</th>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.0</td>
<td>133</td>
<td></td>
</tr>
<tr>
<td>47.8</td>
<td>666.6</td>
<td></td>
</tr>
<tr>
<td>60.8</td>
<td>1333</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>47.8</td>
<td>53.37</td>
</tr>
<tr>
<td>60.8</td>
<td>70.60</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.0</td>
<td>1333</td>
</tr>
<tr>
<td>47.8</td>
<td>666.6</td>
</tr>
<tr>
<td>60.8</td>
<td>1333</td>
</tr>
</tbody>
</table>

**Krasnykh et al. 2002**

<table>
<thead>
<tr>
<th>transpiration method</th>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.85</td>
<td>26.95</td>
<td></td>
</tr>
<tr>
<td>4.85</td>
<td>32.31</td>
<td></td>
</tr>
<tr>
<td>6.85</td>
<td>38.60</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.85</td>
<td>26.95</td>
</tr>
<tr>
<td>4.85</td>
<td>32.31</td>
</tr>
<tr>
<td>6.85</td>
<td>38.60</td>
</tr>
</tbody>
</table>

(Continued)
TABLE 6.1.2.9.1 (Continued)

<table>
<thead>
<tr>
<th></th>
<th>Stull 1947</th>
<th>Ashcroft 1976</th>
<th>Krasnykh et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>summary of lit. data</td>
<td>isoteniscope method</td>
<td>transpiration method</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>75.0</td>
<td>2666</td>
<td>85.63</td>
<td>4246</td>
</tr>
<tr>
<td>90.7</td>
<td>5333</td>
<td>95.35</td>
<td>6330</td>
</tr>
<tr>
<td>100.5</td>
<td>7999</td>
<td>100.2</td>
<td>7905</td>
</tr>
<tr>
<td>114.2</td>
<td>13332</td>
<td>106.95</td>
<td>10566</td>
</tr>
<tr>
<td>134.0</td>
<td>26664</td>
<td>122.67</td>
<td>12883</td>
</tr>
<tr>
<td>1558</td>
<td>53329</td>
<td>117.08</td>
<td>17857</td>
</tr>
<tr>
<td>179.4</td>
<td>101325</td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>–39</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/mmHg</td>
<td>17.95</td>
<td>98.72</td>
</tr>
<tr>
<td>A</td>
<td>6.801</td>
<td>18.95</td>
<td>97.84</td>
</tr>
<tr>
<td>B</td>
<td>1477</td>
<td>20.05</td>
<td>101.6</td>
</tr>
<tr>
<td>C</td>
<td>193.7</td>
<td>21.15</td>
<td>111.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.05</td>
<td>117.44</td>
</tr>
<tr>
<td>∆Hv(kJ mol⁻¹) = 50.1</td>
<td>at 25°C</td>
<td>24.05</td>
<td>133.06</td>
</tr>
<tr>
<td></td>
<td></td>
<td>26.05</td>
<td>153.53</td>
</tr>
<tr>
<td></td>
<td></td>
<td>28.15</td>
<td>175.98</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30.15</td>
<td>204.90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32.15</td>
<td>232.87</td>
</tr>
<tr>
<td></td>
<td></td>
<td>34.15</td>
<td>257.42</td>
</tr>
<tr>
<td></td>
<td></td>
<td>36.15</td>
<td>295.82</td>
</tr>
</tbody>
</table>

FIGURE 6.1.2.9.1 Logarithm of vapor pressure versus reciprocal temperature for α-chlorotoluene.
6.1.2.10 α, α, α-Trichlorotoluene

Common Name: α, α, α-Trichlorotoluene
Synonym: trichloromethylbenzene, benzotrichloride
Chemical Name: α, α, α-Trichlorotoluene
CAS Registry No: 98-07-7
Molecular Formula: C₇H₅Cl₃, C₆H₅CCl₃
Molecular Weight: 195.474
Melting Point (°C):
-4.42 (Lide 2003)
Boiling Point (°C):
221 (Lide 2003)
Density (g/cm³ at 20°C):
1.3723 (20°C, Lide 2003)
Molar Volume (cm³/mol):
142.4 (20°C, calculated-density, Stephenson & Malanowski 1987)
180.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Fusion, ΔH₉ (kJ/mol):
Entropy of Fusion, ΔS₉ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
5.30 (5°C, Riddick et al. 1986)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (45.8, summary of lit. data, Stull 1947)
log (P/mmHg) = –0.2185 × 8869.7/(T/K) + 8.071972, temp range 32–102.2°C (Antoine eq., Weast 1972–73)
34.67 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_kPa) = 6.95923 – 2268.82/(T/K – 28.669); temp range 318–487 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 0.4912 – 2.7285 × 10³/(T/K) + 4.4706·log (T/K) – 1.058 × 10⁻²·(T/K) + 4.7621 × 10⁻⁶·(T/K)²; temp range 268–737 K (Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐw:
2.92 (shake flask, Leo et al. 1979, Hansch & Leo 1979, Hansch et al. 1995; quoted, Sangster 1993)
Octanol/Air Partition Coefficient, log Kₐa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₐc:
Environmental Fate Rate Constants, k, or Half-Lives, tₕ:
Volatilization:
Photolysis:
Oxidation: tₕ = 173.7–1737 h, based on photooxidation half-life in air (Howard et al. 1991)
Hydrolysis: rate constant k = 6.3 × 10⁻² s⁻¹ and tₕ = 19 s at 25°C and pH 7 (Mabey & Mill 1978)
  tₕ = 11 s – 3 min, based on overall hydrolysis rate constants (Howard et al. 1991)
Biodegradation: $t_{1/2}$(aerobic) = 24–168 h, based on limited aqueous screening test data; $t_{1/2} = 96–672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 173.7–1737$ h, based on photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2} = 11$ s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Groundwater: $t_{1/2} = 11$ s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 11$ s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Biota:

### TABLE 6.1.2.10.1
Reported vapor pressures of $\alpha$, $\alpha$, $\alpha$-chlorotoluene at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>45.8</td>
<td>133.3</td>
</tr>
<tr>
<td>73.7</td>
<td>666.6</td>
</tr>
<tr>
<td>87.6</td>
<td>1333</td>
</tr>
<tr>
<td>102.7</td>
<td>2666</td>
</tr>
<tr>
<td>119.8</td>
<td>5333</td>
</tr>
<tr>
<td>130.0</td>
<td>7999</td>
</tr>
<tr>
<td>144.3</td>
<td>13332</td>
</tr>
<tr>
<td>165.6</td>
<td>26664</td>
</tr>
<tr>
<td>189.2</td>
<td>53329</td>
</tr>
<tr>
<td>213.5</td>
<td>101325</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–21.2</td>
</tr>
</tbody>
</table>
6.1.2.11 Pentachlorotoluene

Common Name: Pentachlorotoluene
Synonym:
Chemical Name: pentachlorotoluene
CAS Registry No: 877-11-1
Molecular Formula: C₇H₃Cl₅
Molecular Weight: 264.364
Melting Point (°C):
  224.8 (Lide 2003)
Boiling Point (°C):
  301 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  222.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):

Enthalpy of Fusion, ΔH₅ᵥ (kJ/mol):

Entropy of Fusion, ΔS₅ᵥ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₅ᵥ = 56 J/mol K), F: 0.011 (mp at 224.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  0.028 ± 0.001, 0.047 ± 0.004 (25, 35°C, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kₒw:
  6.20 (calculated as per Hansch & Leo 1979, Oliver & Niimi 1985; Oliver 1987b)
  5.50 (assumed to have approx. the same Kₒw of HCB, Oliver & Charlton 1984)

Octanol/Air Partition Coefficient, log Kₒa:

Bioconcentration Factor, log BCF at 25°C or as indicated:
  3.38–3.86 mean 3.83 (rainbow trout, wet wt., 15°C, steady-state BCF, 7- to 96-d laboratory study, Oliver & Niimi 1985)
  3.83; 4.36 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
  4.45; 3.83 (oligochaete worm; fish, Oliver 1987b)

Sorption Partition Coefficient, log Kₒc:
  5.30 (field data of sediment trap material; Oliver & Charlton 1984)

Environmental Fate Rate Constants, k or Half-Lives, t½:

Half-Lives in the Environment:
  Biotas: elimination t½ = 22 and 26 d, observed and corrected for growth dilution, respectively, in oligochaete worms (Oliver 1987b)
6.1.2.12 \( o \)-Chlorostyrene

![Chemical Structure]

Common Name: \( o \)-Chlorostyrene
Synonym: \( o \)-chlorovinylbenzene, 2-chlorostyrene
Chemical Name: \( o \)-chlorostyrene
CAS Registry No: 2039-87-4
Molecular Formula: C\(_8\)H\(_7\)Cl
Molecular Weight: 138.595
Melting Point (°C):
-63.1 (Lide 2003)
Boiling Point (°C):
188.7 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm\(^3\)):
1.10001, 1.09532 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm\(^3\)/mol):
126.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
153.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
51.03, 40.01 (25°C, bp, Dreisbach 1955)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
127.5 (calculated by formula, Dreisbach 1955)
\[
\log (P/mmHg) = 6.86644 - 1542.1/(198 + t/°C); \text{ temp range } 90-250°C \text{ (Antoine eq. for liquid state, Dreisbach 1955)}
\]
\[
\log (P/kPa) = 6.11856 - 1627.284/(207.112 + t/°C); \text{ temp range } 98.5-154.9°C \text{ (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)}
\]
\[
\log (P_l/kPa) = 5.99134 - 1541.1/(-75.15 + T/K); \text{ temp range } 363-543 K \text{ (Antoine eq., Stephenson & Malanowski 1987)}
\]
Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):
Octanol/Water Partition Coefficient, \( \log K_{OW} \):
Octanol/Air Partition Coefficient, \( \log K_{OA} \):
Bioconcentration Factor, \( \log BCF \) or \( \log K_b \):
Sorption Partition Coefficient, \( \log K_{OC} \):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
Half-Lives in the Environment:
6.1.2.13  \(m\)-Chlorostyrene

\[
\begin{array}{c}
\text{Cl} \\
\text{C}_8\text{H}_7\text{Cl}
\end{array}
\]

Common Name: \(m\)-Chlorostyrene  
Synonym: \(m\)-chlorovinylbenzene, 3-chlorostyrene  
Chemical Name: \(m\)-chlorostyrene  
CAS Registry No: 2039-85-2  
Molecular Formula: \(\text{C}_8\text{H}_7\text{Cl}\)  
Molecular Weight: 138.595  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm\(^3\)):  
\[1.1033 \text{ (20°C, Lide 2003)}\]  
Molar Volume (cm\(^3\)/mol):  
\[124.1 \text{ (20°C, calculated-density, Stephenson & Malanowski 1987)}\]  
\[153.9 \text{ (calculated-Le Bas method at normal boiling point)}\]  
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):  
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):  
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):  
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):  
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), \(F\):  
Water Solubility (g/m\(^3\) or mg/L at 25°C):  
Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
\[133.3^* \text{ (25.3°C, summary of literature data, Stull 1947)}\]  
\[148.06 \text{ (interpolated-Antoine eq., Stephenson & Malanowski 1987)}\]  
\[
\log (P_l/\text{kPa}) = 6.83847 – 2156.77/(-16.882 + T/K); \text{ temp range 298–463 K (Antoine eq., Stephenson & Malanowski 1987)}
\]  
Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):  
Octanol/Water Partition Coefficient, log \(K_{ow}\):  
Octanol/Air Partition Coefficient, log \(K_{oa}\):  
Bioconcentration Factor, log BCF or log \(K_b\):  
Sorption Partition Coefficient, log \(K_{OC}\):  
Environmental Fate Rate Constant, \(k\), and Half-Lives, \(t_{1/2}\):  
Half-Lives in the Environment:
<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.3</td>
<td>133.3</td>
</tr>
<tr>
<td>51.3</td>
<td>666.6</td>
</tr>
<tr>
<td>65.2</td>
<td>1333</td>
</tr>
<tr>
<td>80.0</td>
<td>2666</td>
</tr>
<tr>
<td>96.5</td>
<td>5333</td>
</tr>
<tr>
<td>107.2</td>
<td>7999</td>
</tr>
<tr>
<td>121.1</td>
<td>13332</td>
</tr>
<tr>
<td>142</td>
<td>26664</td>
</tr>
<tr>
<td>165.7</td>
<td>53329</td>
</tr>
<tr>
<td>190</td>
<td>101325</td>
</tr>
</tbody>
</table>
6.1.2.14  \( p \)-Chlorostyrene

Common Name: \( p \)-Chlorostyrene  
Synonym: \( p \)-chlorovinylbenzene, 4-chlorostyrene  
Chemical Name: \( p \)-chlorostyrene  
CAS Registry No: 1073-67-2  
Molecular Formula: \( \text{C}_8\text{H}_7\text{Cl} \)  
Molecular Weight: 138.595  

Melting Point (°C):  
\(-15.9\)  
(Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)  
Boiling Point (°C):  
192.0  
(Dreisbach 1955, Lide 2003)  

Density (g/cm\(^3\)):  
1.08682, 1.08214 (20°C, 25°C, Dreisbach 1955)  
1.0868 (20°C, Lide 2003)  

Molar Volume (cm\(^3\)/mol):  
127.5 (20°C, calculated-density, Stephenson & Malanowski 1987)  
153.9 (calculated-Le Bas method at normal boiling point)  

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
51.11, 40.07 (25°C, bp, Dreisbach 1955)  

Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):  

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):  

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):  

Fugacity Ratio at 25°C, \( F \): 1.0  

Water Solubility (g/m\(^3\) or mg/L at 25°C):  

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
133.3* (28.0°C, summary of literature data, temp range 28.0–191.0°C, Stull 1947)  
6287* (100.91°C, ebulliometry, measured range 100.91–127.27°C, Dreisbach & Shrader 1949)  
116.3 (calculated by formula, Dreisbach 1955)  
log (P/mmHg) = 6.84248 – 1545.0/(198 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)  
log (P/kPa) = 9.18404 – 4186.871/(398.256 + t/°C); temp range 100.9–127.27°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)  
log (P/kPa) = 5.96738 – 1545.0/(–75.15 + T/K); temp range 363–523 K (Antoine eq., Stephenson & Malanowski 1987)  

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):  

Octanol/Water Partition Coefficient, log \( K_{ow} \):  
3.66 (estimated, Kaiser 1987)  

Octanol/Air Partition Coefficient, log \( K_{oa} \):  

Bioconcentration Factor, log BCF or log \( K_b \):  

Sorption Partition Coefficient, log \( K_{oc} \):  

Environmental Fate Rate Constant, \( k \), and Half-Lives, \( t_{1/2} \):  
Half-Lives in the Environment:
TABLE 6.1.2.14.1
Reported vapor pressures of p-chlorostyrene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.0</td>
<td>133.3</td>
<td>100.91</td>
<td>6287</td>
</tr>
<tr>
<td>54.5</td>
<td>666.6</td>
<td>106.09</td>
<td>7605</td>
</tr>
<tr>
<td>67.5</td>
<td>1333</td>
<td>109.97</td>
<td>8851</td>
</tr>
<tr>
<td>82.0</td>
<td>2666</td>
<td>113.76</td>
<td>10114</td>
</tr>
<tr>
<td>98.0</td>
<td>5333</td>
<td>127.27</td>
<td>16500</td>
</tr>
<tr>
<td>105.8</td>
<td>7999</td>
<td></td>
<td></td>
</tr>
<tr>
<td>122.0</td>
<td>13332</td>
<td></td>
<td></td>
</tr>
<tr>
<td>143.5</td>
<td>26664</td>
<td></td>
<td></td>
</tr>
<tr>
<td>166.0</td>
<td>53329</td>
<td></td>
<td></td>
</tr>
<tr>
<td>191.0</td>
<td>101325</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 6.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for p-chlorostyrene.
6.1.2.15 Octochlorostyrene

[Chemical structure image]

Common Name: Octochlorostyrene
Synonym:
Chemical Name: octachlorostyrene
CAS Registry No: 29082-74-4
Molecular Formula: C₈Cl₈
Molecular Weight: 379.710
Melting Point (°C):
  99 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  300.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
Enthalpy of Fusion, ∆Hₛ (kJ/mol):
Entropy of Fusion, ∆Sₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₛ = 56 J/mol K), F: 0.188 (mp at 99°C)
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
  22.9(20°C, calculated-bond contribution method, Meylan & Howard 1991)
Octanol/Water Partition Coefficient, log Kₐw:
  6.29 (HPLC-RT correlation, Veith et al.1979b)
  6.20 (HPLC-RT correlation, Veith et al. 1979a)
Bioconcentration Factor, log BCF:
  4.52 (fathead minnow, 32-d exposure, Veith et al. 1979b)
  2.91–3.91, mean 3.91 (rainbow trout, 15°C, wet wt., steady-state BCF on 7- to 96-d laboratory study; Oliver & Niimi 1985)
  5.38; 6.15 (rainbow trout, calculated-Kₐw, Lake Ontario field BCF, Oliver & Niimi 1985)
  4.49; 3.91 (oligochaete worms; fish, Oliver 1987b)
Sorption Partition Coefficient, log Kₐc:
  6.10 (field data of sediment trap material, Oliver & Charlton 1984)
  5.90–7.30; 6.60 (suspended sediment: range; mean, Oliver 1987a)
  6.30 (algae > 50 μm, mean, Oliver 1987a)
Environmental Fate Rate Constants, k, or Half-Lives, tᵢₑ:
Half-Lives in the Environment:
  Biota: elimination tᵢₑ = 71 d, observed and tᵢₑ = 100 d, corrected for growth dilution in worms (8°C, Oliver 1987).
6.1.3  FLUOROBENZENES

6.1.3.1  Fluorobenzene

Common Name: Fluorobenzene
Synonym: phenyl fluoride
Chemical Name: fluorobenzene, phenyl fluoride
CAS Registry No: 462-06-6
Molecular Formula: C\textsubscript{6}H\textsubscript{5}F
Molecular Weight: 96.102

Melting Point (°C): -42.18 (Lide 2003)
Boiling Point (°C): 84.73 (Riddick et al. 1986; Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C): 1.0225 (Horvath 1982; Lide 2003), 1.0131 (30°C, Riddick et al. 1986)
Molar Volume (cm\textsuperscript{3}/mol): 94.4 (Stephenson & Malanowski 1987; Wang et al. 1992), 101.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 11.305 (quoted, Riddick et al. 1986)
Entropy of Fusion, \(\Delta S_f\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):
1540 (30°C, shake flask-IR, Gross et al. 1933)
1550 (shake flask-UV spectrophotometer, Andrews & Keefer 1950)
1296 (Deno & Berklheimer 1960)
922 (shake flask-GC, Jones et al. 1977/1978)
189.3* (shake flask-GC, measured range 5–45°C, Nelson & Smit 1978)
1559 (Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
1540 (27.5°C, recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
1530 (30°C, Riddick et al. 1986)
1700*, 1550 (19.2°C, 29.7°C, shake flask-GC/TC, measured range 0–80°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):
10246* (24.9°C, Ramsay-Young method, measured range –17.85 to 83.85°C, Young 1889)
7999* (19.6°C, summary of literature data, temp range –43.4 to 84.7°C, Stull 1947)
19920* (39.4°C, comparative ebulliometry, measured range 39.4–120.5°C, Scott et al. 1956)
\[
\log (P/mmHg) = 6.95208 - 1248.083/(221.827 + t/°C); \text{ temp range 34.5–120.5°C (Antoine eq., comparative ebulliometry, Scott et al. 1956)}
\]
\[
\log (P/mmHg) = [–0.2185 \times 7980.4/(T/K)] + 7.699237; \text{ temp range –43.4–279.3°C (Antoine eq., Weast 1972–73)}
\]
\[
10200 (interpolated-Antoine eq., Boublik et al. 1973, 1984)
\]
\[
\log (P/mmHg) = 7.18703 - 1381.828/(235.563 + t/°C); \text{ temp range –17.85 to 83.85°C (Antoine eq. from reported explt. data, Boublik et al. 1973)}
\]
\[
\log (P/kPa) = 6.31155 – 1381.646/(235.548 + t/°C); \text{ temp range –17.85 to 83.85°C (Antoine eq. from reported explt. data, Boublik et al. 1984)}
\]
log (P/mmHg) = 7.1870 – 1381.8/(235.6 + t°C); temp range –18 to 84°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 6.07698 – 1248.083/(221.827 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 10480 (Riddick et al. 1986)
log (P/L/kPa) = 6.07234 – 1245.564/(–51.587 + T/K); temp range 312–394 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/L/kPa) = 5.4113 – 1398.61/(–31.295 + T/K); temp range 358–530 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/L/kPa) = 6.14135 – 1291.116/(–45.664 + T/K); temp range 373–419 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/L/kPa) = 6.37857 – 1478.807/(–18.847 + T/K); temp range 414–501 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/L/kPa) = 7.59182 – 2876.741/(171.093 + T/K); temp range 497–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P/L/kPa) = –5.4849 – 1.8597 × 10³/(T/K) + 7.1515·log (T/K) – 1.6467 × 10⁻²·(T/K) + 9.2622 × 10⁻⁶·(T/K)², temp range 231–560 K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

632 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log Kₗₒw:

2.27 (shake flask-AS, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)
2.28 (calculated-fragment const., Rekker 1977)
2.27 (recommended, Sangster 1989, 1993)
2.26 (centrifugal partition chromatography, El Tayar et al. 1991)
2.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₗₒₐ:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Kₗₒₐ:

Environmental Fate Rate Constants, k, and Half-Lives, t₁/₂:

Vaporization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order reaction rate constants, kₒH for reaction with OH radical, kₒN₃ with NO₃ radical and kₒO₃ with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

kₒH(calc) = 2.6 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, kₒH(obs) = 0.54 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)

kₒH* = (6.31 ± 0.84) × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

kₒH = 6.31 ± 2 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹; k(soln) = 1.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

kₒH = 6.90 ± 7 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, independent of temperature over the range 234–303 K (Atkinson 1989)

kₒH(calc) = 1.08 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:
TABLE 6.1.3.1.1
Reported aqueous solubilities of fluorobenzene at various temperatures

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-interferometer</td>
<td>shake flask-GC</td>
<td>shake flask-GC/TC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>S/g·m⁻³</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>30</td>
<td>1540</td>
<td>5</td>
<td>118.4</td>
</tr>
<tr>
<td>25</td>
<td>189.3</td>
<td>9.5</td>
<td>1660</td>
</tr>
<tr>
<td>35</td>
<td>336</td>
<td>29.7</td>
<td>1700</td>
</tr>
<tr>
<td>45</td>
<td>512</td>
<td>39.6</td>
<td>1530</td>
</tr>
<tr>
<td>Andrews &amp; Keefer 1950</td>
<td>shake flask-UV</td>
<td>60.1</td>
<td>1900</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>1550</td>
<td>70</td>
<td>1901</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80</td>
<td>1880</td>
</tr>
</tbody>
</table>

FIGURE 6.1.3.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for fluorobenzene.
TABLE 6.1.3.1.2
Reported vapor pressures of fluorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/\text{K}} \quad (1) \\
\ln P = A - \frac{B}{T/\text{K}} \quad (1a) \\
\log P = A - \frac{B}{(C + t/\degree \text{C})} \quad (2) \\
\ln P = A - \frac{B}{(C + t/\degree \text{C})} \quad (2a) \\
\log P = A - \frac{B}{T/\text{K}} - C\log (T/\text{K}) \quad (3) \\
\log P = A - \frac{B}{T/\text{K}} - C\log (T/\text{K}) \quad (4)
\]

Young 1889

<table>
<thead>
<tr>
<th>t/\degree \text{C}</th>
<th>P/Pa</th>
<th>Stull 1947</th>
<th>summary of literature data</th>
</tr>
</thead>
<tbody>
<tr>
<td>–17.85</td>
<td>927</td>
<td>–43.4</td>
<td>133.3</td>
</tr>
<tr>
<td>–5.95</td>
<td>1980</td>
<td>–22.8</td>
<td>666.6</td>
</tr>
<tr>
<td>0.15</td>
<td>2806</td>
<td>–12.4</td>
<td>1333</td>
</tr>
<tr>
<td>4.7</td>
<td>3613</td>
<td>–1.20</td>
<td>2666</td>
</tr>
<tr>
<td>10.65</td>
<td>5000</td>
<td>11.5</td>
<td>5333</td>
</tr>
<tr>
<td>16.75</td>
<td>6873</td>
<td>19.6</td>
<td>7999</td>
</tr>
<tr>
<td>19.5</td>
<td>7866</td>
<td>30.4</td>
<td>13332</td>
</tr>
<tr>
<td>24.9</td>
<td>10246</td>
<td>47.2</td>
<td>26664</td>
</tr>
<tr>
<td>30.35</td>
<td>12999</td>
<td>65.7</td>
<td>53329</td>
</tr>
<tr>
<td>36.05</td>
<td>16759</td>
<td>84.7</td>
<td>101325</td>
</tr>
<tr>
<td>42.05</td>
<td>21558</td>
<td></td>
<td></td>
</tr>
<tr>
<td>49.6</td>
<td>29317</td>
<td>mp/\degree \text{C}</td>
<td>–42.1</td>
</tr>
<tr>
<td>56.2</td>
<td>37610</td>
<td></td>
<td></td>
</tr>
<tr>
<td>62.75</td>
<td>47889</td>
<td></td>
<td></td>
</tr>
<tr>
<td>71</td>
<td>63995</td>
<td></td>
<td></td>
</tr>
<tr>
<td>78.75</td>
<td>82473</td>
<td></td>
<td></td>
</tr>
<tr>
<td>83.85</td>
<td>97378</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

complete set of data see ref.

FIGURE 6.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for fluorobenzene.
6.1.3.2 1,2-Difluorobenzene

Common Name: 1,2-Difluorobenzene
Synonym:  o-difluorobenzene
Chemical Name: 1,2-Difluorobenzene
CAS Registry No: 367-11-3
Molecular Formula: C₆H₄F₂
Molecular Weight: 114.093
Melting Point (°C):
  -47.1 (Lide 2003)
Boiling Point (°C):
  94 (Lide 2003)
Density (g/cm³ at 20°C):
  1.158 (Dean 1992)
Molar Volume (cm³/mol):
  99.2 (calculated-density, Stephenson & Malanowski 1987)
  106.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
Enthalpy of Fusion, ∆Hₚ (kJ/mol):
Entropy of Fusion, ∆Sₚ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  log (P/kPa) = 6.12360 – 1297.243/(211.103 + t/°C); temp range 31.2–130°C (Antoine eq. derived from experimental data of Scott et al.1963, Boublik et al. 1984)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  713 (computer value, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log Kₐw:
  2.59 (calculated-fragment const., Valvani & Yalkowsky 1980)
  2.58 (calculated-fragment const., Yalkowsky et al. 1983)
  2.56 (calculated-molar volume correlation, Wang et al. 1992)
  2.43 (calculated, Müller & Klein 1992)
  2.37 (recommended, Hansch et al. 1995)
  2.25; 2.33 (predicted; calc-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Kₐa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₐc:
Environmental Fate Rate Constants, k or Half-Lives, t½:
  Half-Lives in the Environment:
TABLE 6.1.3.2.1
Reported vapor pressures of 1,2-difluorobenzene at various temperatures

Scott et al. 1963
comparative ebulliometry

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.168</td>
<td>9582</td>
<td>111.903</td>
<td>169053</td>
</tr>
<tr>
<td>33.916</td>
<td>10884</td>
<td>117.980</td>
<td>198530</td>
</tr>
<tr>
<td>36.668</td>
<td>12335</td>
<td>124.099</td>
<td>232088</td>
</tr>
<tr>
<td>39.436</td>
<td>13950</td>
<td>130.256</td>
<td>270111</td>
</tr>
<tr>
<td>42.210</td>
<td>15740</td>
<td>124.099</td>
<td>232088</td>
</tr>
<tr>
<td>44.996</td>
<td>17725</td>
<td>mp/K</td>
<td>226.0148</td>
</tr>
<tr>
<td>47.803</td>
<td>19920</td>
<td>bp/K</td>
<td>367.07</td>
</tr>
<tr>
<td>53.423</td>
<td>25007</td>
<td>∆H_fus = 11.045 kJ/mol</td>
<td></td>
</tr>
<tr>
<td>59.084</td>
<td>31160</td>
<td>∆H_v = 36.11 kJ/mol</td>
<td></td>
</tr>
<tr>
<td>64.787</td>
<td>38547</td>
<td>Antoine eq.</td>
<td></td>
</tr>
<tr>
<td>70.530</td>
<td>47359</td>
<td>∆H_fus = 11.045 kJ/mol</td>
<td></td>
</tr>
<tr>
<td>68.142</td>
<td>57803</td>
<td>P/mmHg</td>
<td></td>
</tr>
<tr>
<td>82.142</td>
<td>70109</td>
<td>A</td>
<td>7.00003</td>
</tr>
<tr>
<td>88.009</td>
<td>84525</td>
<td>B</td>
<td>1298.053</td>
</tr>
<tr>
<td>93.921</td>
<td>101325</td>
<td>C</td>
<td>221.197</td>
</tr>
<tr>
<td>99.874</td>
<td>120798</td>
<td></td>
<td></td>
</tr>
<tr>
<td>105.869</td>
<td>143268</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 6.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-difluorobenzene.
6.1.3.3 1,3-Difluorobenzene

Common Name: 1,3-Difluorobenzene
Synonym: m-difluorobenzene
Chemical Name: 1,3-Difluorobenzene
CAS Registry No: 372-18-9
Molecular Formula: C₆H₄F₂
Molecular Weight: 114.093
Melting Point (°C): -69.12 (Lide 2003)
Boiling Point (°C): 82.6 (Lide 2003)
Density (g/cm³ at 20°C):
1.1552 (18°C, Horvath 1982)
1.1572 (Lide 2003)
Molar Volume (cm³/mol):
98.6 (20°C, calculated-density, Stephenson & Malanowski 1987, Ruelle & Kesselring 1997)
106.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Fusion, ΔH₉₅ (kJ/mol):
Entropy of Fusion, ΔS₉₅ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₒw:
2.58 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
2.56 (calculated-molar volume correlation, Wang et al. 1992)
2.43 (calculated, Müller & Klein 1992)
2.26; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Kₒa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₒc:
Environmental Fate Rate Constants, k or Half-Lives, t½:
Half-Lives in the Environment:
**TABLE 6.1.3.3.1**  
Reported vapor pressures of 1,3-difluorobenzene at various temperatures  

Osborn & Scott 1980  

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>38.184</td>
<td>19924</td>
<td>88.808</td>
<td>120800</td>
</tr>
<tr>
<td>43.646</td>
<td>25014</td>
<td>94.641</td>
<td>143270</td>
</tr>
<tr>
<td>49.148</td>
<td>31167</td>
<td>100.511</td>
<td>169050</td>
</tr>
<tr>
<td>54.692</td>
<td>38553</td>
<td>106.425</td>
<td>198540</td>
</tr>
<tr>
<td>60.273</td>
<td>47363</td>
<td>112.378</td>
<td>232090</td>
</tr>
<tr>
<td>65.898</td>
<td>57806</td>
<td>118.373</td>
<td>270120</td>
</tr>
<tr>
<td>71.564</td>
<td>70112</td>
<td></td>
<td></td>
</tr>
<tr>
<td>77.272</td>
<td>84528</td>
<td></td>
<td>data fitted to a 4-constant</td>
</tr>
<tr>
<td>83.02</td>
<td>101325</td>
<td></td>
<td>vapor pressure eq.</td>
</tr>
</tbody>
</table>

**FIGURE 6.1.3.3.1** Logarithm of vapor pressure versus reciprocal temperature for 1,3-difluorobenzene.
6.1.3.4  1,4-Difluorobenzene

Common Name: 1,4-Difluorobenzene
Synonym: p-difluorobenzene
Chemical Name: 1,4-Difluorobenzene
CAS Registry No: 540-36-3
Molecular Formula: C₆H₄F₂
Molecular Weight: 114.093
Melting Point (°C):
-23.55  (Lide 2003)
Boiling Point (°C):
89  (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
97.4  (20°C, calculated-density, Stephenson & Malanowski 1987)
106.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hv (kJ/mol):
Enthalpy of Fusion, ∆Hfus (kJ/mol):
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
1222  (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9577*  (27.25°C, comparative ebulliometry, measured temp range 300.4–397.7 K, Osborn & Scott 1980)
Henry’s Law Constant (Pa m³/mol at 25°C):
776  (computer value, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log Kow:
2.58  (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
2.43  (calculated, Müller & Klein 1992)
2.84  (calculated-molar volume, Wang et al. 1992)
2.24; 2.33  (predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Half-Lives in the Environment:
TABLE 6.1.3.4.1
Reported vapor pressures of 1,4-difluorobenzene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.248</td>
<td>9577</td>
<td>84.078</td>
<td>84528</td>
</tr>
<tr>
<td>30.95</td>
<td>10789</td>
<td>89.886</td>
<td>101325</td>
</tr>
<tr>
<td>33.658</td>
<td>12331</td>
<td>95.727</td>
<td>120800</td>
</tr>
<tr>
<td>36.376</td>
<td>13944</td>
<td>101.611</td>
<td>143270</td>
</tr>
<tr>
<td>39.101</td>
<td>15736</td>
<td>107.535</td>
<td>169050</td>
</tr>
<tr>
<td>41.837</td>
<td>17721</td>
<td>113.503</td>
<td>198540</td>
</tr>
<tr>
<td>44.588</td>
<td>19924</td>
<td>119.507</td>
<td>232090</td>
</tr>
<tr>
<td>50.109</td>
<td>25104</td>
<td>125.552</td>
<td>270120</td>
</tr>
<tr>
<td>55.671</td>
<td>31167</td>
<td></td>
<td></td>
</tr>
<tr>
<td>61.273</td>
<td>38553</td>
<td>data fitted to a 4-constant vapor pressure eq.</td>
<td></td>
</tr>
<tr>
<td>66.910</td>
<td>47363</td>
<td></td>
<td></td>
</tr>
<tr>
<td>72.593</td>
<td>57806</td>
<td></td>
<td></td>
</tr>
<tr>
<td>78.319</td>
<td>70112</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 6.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-difluorobenzene.
6.1.3.5 1,2,4-Trifluorobenzene

Common Name: 1,2,4-Trifluorobenzene
Synonym:
Chemical Name: 1,2,4-trifluorobenzene
CAS Registry No: 367-23-7
Molecular Formula: C₆H₃F₃
Molecular Weight: 132.083
Melting Point (°C):
Boiling Point (°C):
  90  (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
  111.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
  2.52  (HPLC-RT correlation, Garst 1984, quoted, Sangster 1993)
  2.41  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log KoA:
Bioconcentration Factor, log BCF or log Kb:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
6.1.3.6 1,3,5-Trifluorobenzene

F

F

F

Common Name: 1,3,5-Trifluorobenzene
Synonym:
Chemical Name: 1,3,5-trifluorobenzene
CAS Registry No: 372-38-3
Molecular Formula: C\textsubscript{6}H\textsubscript{3}F\textsubscript{3}
Molecular Weight: 132.083

Melting Point (°C):
-5.5 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
75.4 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm\textsuperscript{3}):
103.4 (calculated-density, Stephenson & Malanowski 1987)
111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):

Enthalpy of Sublimation, $\Delta H_{sub}$ (kJ/mol):

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
139.68* (25.21°C, static system-Hg manometer, measured range 6.18–50°C, Findlay 1969)

log (P/mmHg) = 6.91873 – 1196.385/(219.01 + t/°C); temp range 6.18–50°C (Hg manometer, Findlay 1969)

log (P L/kPa) = 6.04363 – 1198.385/(-54.131 + T/K); temp range 279–350 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{ow}$:

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF or log $K_{bi}$:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:
## TABLE 6.1.3.6.1
Reported vapor pressures of 1,3,5-trifluorobenzene at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.18</td>
<td>5385</td>
<td>25.24</td>
<td>13965</td>
<td>46.97</td>
<td>35156</td>
</tr>
<tr>
<td>6.19</td>
<td>5389</td>
<td>29.98</td>
<td>17331</td>
<td>46.97</td>
<td>35168</td>
</tr>
<tr>
<td>10.03</td>
<td>6615</td>
<td>29.98</td>
<td>17339</td>
<td>49.98</td>
<td>39.453</td>
</tr>
<tr>
<td>15.01</td>
<td>8530</td>
<td>35.15</td>
<td>21679</td>
<td>49.99</td>
<td>39.462</td>
</tr>
<tr>
<td>15.01</td>
<td>8534</td>
<td>35.25</td>
<td>21806</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.99</td>
<td>10915</td>
<td>35.39</td>
<td>21846</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.99</td>
<td>10911</td>
<td>40.05</td>
<td>26654</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.49</td>
<td>11.202</td>
<td>40.11</td>
<td>26704</td>
<td>A</td>
<td>6.91873</td>
</tr>
<tr>
<td>20.53</td>
<td>11210</td>
<td>43.85</td>
<td>31019</td>
<td>B</td>
<td>1196.385</td>
</tr>
<tr>
<td>22.79</td>
<td>12468</td>
<td>43.94</td>
<td>31188</td>
<td>C</td>
<td>219.019</td>
</tr>
<tr>
<td>25.21</td>
<td>13968</td>
<td>44.2</td>
<td>31463</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\log P = A - B/(C + t/°C)
\]

### FIGURE 6.1.3.6.1
Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trifluorobenzene.
6.1.3.7 1,2,3,4-Tetrafluorobenzene

Common Name: 1,2,3,4-Tetrafluorobenzene
Synonym:
Chemical Name: 1,2,3,4-tetrafluorobenzene
CAS Registry No: 551-62-2
Molecular Formula: C₆H₂F₄
Molecular Weight: 150.074
Melting Point (°C):
   –42  (Stephenson & Malanowski 1987)
Boiling Point (°C):
   94.3  (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
   105.5  (calculated-density, Stephenson & Malanowski 1987)
   116.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
   33.0  (Ambrose et al. 1975)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   6545*  (24.82°C, static-system-Hg manometer, Findlay 1969)
   \( \log (P/mmHg) = 7.19386 - 1396.067/(228.837 + t/°C) \); temp range 6.05–49.87°C (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
   6509*  (extrapolated from ebulliometric measurements, Ambrose et al. 1975)
   \( \log (P/kPa) = 6.15854 - 1291.080/(-50.617 + T/K) \); temperature range 300.8–367.51(normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
   \( \log (P/kPa) = 6.16107 - 1292.550/(-56.453 + T/K) \); temperature range 300.8–391.65 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
   \( \log (P/kPa) = 6.21410 - 1341.655/(223.721 + t/°C) \); temp range 24.78–84.98°C (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)
   \( \log (P/kPa) = 6.15952 - 1291.522/(216.58 + t/°C) \); temp range 27.65–118.5°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)
   \( \log (P/kPa) = 6.31876 - 1396.067/(-44.277 + T/K) \); temp range 279–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   \( \log (P/kPa) = 6.16042 - 1292.174/(-56.495 + T/K) \); temp range 300–392 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, \( \log K_{ow} \):
Octanol/Air Partition Coefficient, \( \log K_{oa} \):
Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):
Sorption Partition Coefficient, \( \log K_{OC} \):

© 2006 by Taylor & Francis Group, LLC
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \); Half-Lives in the Environment:

**TABLE 6.1.3.7.1**

Reported vapor pressures of 1,2,3,4-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations:

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \text{Hg manometer} )</th>
<th>( \text{ebulliometry} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T/K )</td>
<td>( P/Pa )</td>
<td>( T/K )</td>
</tr>
<tr>
<td>6.05</td>
<td>2385</td>
<td>44.01</td>
</tr>
<tr>
<td>6.06</td>
<td>2377</td>
<td>46.91</td>
</tr>
<tr>
<td>10.36</td>
<td>3041</td>
<td>46.91</td>
</tr>
<tr>
<td>15.21</td>
<td>3970</td>
<td>48.82</td>
</tr>
<tr>
<td>20.64</td>
<td>5277</td>
<td>48.83</td>
</tr>
<tr>
<td>24.82</td>
<td>6545</td>
<td>49.84</td>
</tr>
<tr>
<td>24.82</td>
<td>6547</td>
<td>49.87</td>
</tr>
<tr>
<td>29.98</td>
<td>8433</td>
<td></td>
</tr>
<tr>
<td>29.99</td>
<td>8433</td>
<td>eq. 2 P/mmHg</td>
</tr>
<tr>
<td>35.05</td>
<td>10722 A</td>
<td>7.19386</td>
</tr>
<tr>
<td>35.06</td>
<td>10722 B</td>
<td>1396.067</td>
</tr>
<tr>
<td>40.07</td>
<td>13438 C</td>
<td>228.984</td>
</tr>
<tr>
<td>40.07</td>
<td>13439</td>
<td></td>
</tr>
<tr>
<td>43.99</td>
<td>15904</td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.3.7.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetrafluorobenzene.
6.1.3.8 1,2,3,5-Tetrafluorobenzene

Common Name: 1,2,3,5-Tetrafluorobenzene
Synonym: 
Chemical Name: 1,2,3,5-tetrafluorobenzene
CAS Registry No: 2367-82-0
Molecular Formula: C₆H₂F₄
Molecular Weight: 150.074
Melting Point (°C): 
−46.25 (Lide 2003)
Boiling Point (°C): 
84.4 (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
107.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
116.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
32.1 (Ambrose et al. 1975)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9770* (24.81°C, static method-Hg manometer, measured range 6.08–50°C, Findlay 1969)
log (P/mmHg) = 7.07758 − 1290.984/222.855 + t/°C); temp range 6.08–49.83°C (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
9801* (interpolated from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.15414 − 1255.781/(−54.898 + T/K); temperature range 287.6–357.61 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.1500 – 1253.771/(−55.168 + T/K); temperature range 287–382 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.12070 – 1250.027/(217.903 + t/°C); temp range 14.44–108.37°C (Antoine eq. derived from Findlay 1969 data, Boublík et al. 1984)
log (P/kPa) = 6.1500 − 1253.079/(217.903 + t/°C); temp range 14.44−108.37°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublík et al. 1984)
log (P/kPa) = 6.15119 − 1253.771/(−55.168 + T/K); temperature range 287–382 K (Antoine eq.-II from Ambrose et al. 1975, Stephenson & Malanowski 1987)
log (P/kPa) = 6.15119 − 1253.771/(−55.168 + T/K); temperature range 287–382 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.24644 − 1317.349/(−46.898 + T/K); temp range 385–416 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log KOW:
Octanol/Air Partition Coefficient, log KoA:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_\text{½}:
Half-Lives in the Environment:

### TABLE 6.1.3.8.1
Reported vapor pressures of 1,2,3,5-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.05</td>
<td>2385</td>
<td>48.82</td>
<td>19620</td>
</tr>
<tr>
<td>6.06</td>
<td>2377</td>
<td>48.83</td>
<td>19621</td>
</tr>
<tr>
<td>10.36</td>
<td>3041</td>
<td>49.84</td>
<td>20380</td>
</tr>
<tr>
<td>15.21</td>
<td>3970</td>
<td>49.87</td>
<td>20428</td>
</tr>
<tr>
<td>20.64</td>
<td>5277</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24.82</td>
<td>6545 eq. 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24.82</td>
<td>6547 A</td>
<td>7.07758</td>
<td></td>
</tr>
<tr>
<td>29.98</td>
<td>8433 B</td>
<td>1290.984</td>
<td></td>
</tr>
<tr>
<td>29.99</td>
<td>8433 C</td>
<td>223.855</td>
<td></td>
</tr>
<tr>
<td>35.05</td>
<td>10722</td>
<td></td>
<td></td>
</tr>
<tr>
<td>35.06</td>
<td>10722</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40.07</td>
<td>13438</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40.07</td>
<td>13439</td>
<td></td>
<td></td>
</tr>
<tr>
<td>43.99</td>
<td>15904</td>
<td></td>
<td></td>
</tr>
<tr>
<td>44.01</td>
<td>15919</td>
<td></td>
<td></td>
</tr>
<tr>
<td>46.91</td>
<td>18024</td>
<td></td>
<td></td>
</tr>
<tr>
<td>46.91</td>
<td>18024</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>287.593</td>
<td>5719</td>
<td>357.291</td>
<td>100305</td>
</tr>
<tr>
<td>291.414</td>
<td>6987</td>
<td>357.743</td>
<td>101755</td>
</tr>
<tr>
<td>295.169</td>
<td>8457</td>
<td>362.582</td>
<td>118237</td>
</tr>
<tr>
<td>298.091</td>
<td>9773</td>
<td>366.716</td>
<td>133926</td>
</tr>
<tr>
<td>303.399</td>
<td>12598</td>
<td>371.603</td>
<td>154528</td>
</tr>
<tr>
<td>307.963</td>
<td>15541</td>
<td>376.423</td>
<td>177795</td>
</tr>
<tr>
<td>312.406</td>
<td>18930</td>
<td>381.524</td>
<td>203.907</td>
</tr>
<tr>
<td>314.635</td>
<td>20846</td>
<td></td>
<td></td>
</tr>
<tr>
<td>317.751</td>
<td>24802</td>
<td></td>
<td></td>
</tr>
<tr>
<td>324.852</td>
<td>31779</td>
<td></td>
<td></td>
</tr>
<tr>
<td>329.202</td>
<td>37666</td>
<td></td>
<td></td>
</tr>
<tr>
<td>334.506</td>
<td>46007 eq. 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>338.643</td>
<td>53501 A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>343.224</td>
<td>62911 B</td>
<td></td>
<td></td>
</tr>
<tr>
<td>347.715</td>
<td>73374 C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>352.951</td>
<td>87269</td>
<td></td>
<td></td>
</tr>
<tr>
<td>356.719</td>
<td>98504</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.3.8.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetrafluorobenzene.
6.1.3.9 1,2,4,5-Tetrafluorobenzene

Common Name: 1,2,4,5-Tetrafluorobenzene
Synonym:
Chemical Name: 1,2,4,5-tetrafluorobenzene
CAS Registry No: 327-54-8
Molecular Formula: C₆H₂F₄
Molecular Weight: 150.074
Melting Point (°C):
3.88 (Lide 2003)
Boiling Point (°C):
90.2 (Lide 2003)
Density (g/cm³ at 20°C):
1.4255 (Lide 2003)
Molar Volume (cm³/mol):
105.3 (20°C, calculated-density)
105.4 (calculated-density, Stephenson & Malanowski 1987)
116.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔΗᵥ (kJ/mol):
32.9 (Ambrose et al. 1975)
Enthalpy of Fusion, ΔΗ₆₅₅ (kJ/mol):
Entropy of Fusion, ΔS₆₅₅ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7556* (interpolated from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17340 – 1277.452/(–56.889 + T/K); temp range 293.2–363.413 (normal bp K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17788 – 1279.904/(–56.642 + T/K); temp range 293.2–387.6 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)
log (P/kPa) = 6.17439 – 1277.918/(216.289 + t/°C); temp range 20.05–114.42°C (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)
log (P/L/kPa) = 6.17614 – 1278.93/(–56.748 + T/K); temp range 293–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/L/kPa) = 6.42009 – 1454.406/(–33.675 + T/K); temp range 390–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/L/kPa) = 7.88521 – 3090.851/(174.387 + T/K); temp range 488–543 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒ₆₅₅:
Octanol/Air Partition Coefficient, log Kₒ₈₅₅:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₒ₆₅₅:
Environmental Fate Rate Constants, k and Half-Lives, t½:
Half-Lives in the Environment:
### TABLE 6.1.3.9.1
Reported vapor pressures of 1,2,4,5-tetrafluorobenzene at various temperatures:

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.198</td>
<td>5855</td>
<td>363.049</td>
<td>100177</td>
</tr>
<tr>
<td>296.489</td>
<td>6944</td>
<td>363.591</td>
<td>101.896</td>
</tr>
<tr>
<td>300.519</td>
<td>8505</td>
<td>368.237</td>
<td>117566</td>
</tr>
<tr>
<td>303.459</td>
<td>9822</td>
<td>372.427</td>
<td>133286</td>
</tr>
<tr>
<td>308.374</td>
<td>12399</td>
<td>377.572</td>
<td>154790</td>
</tr>
<tr>
<td>313.302</td>
<td>15524</td>
<td>382.398</td>
<td>177330</td>
</tr>
<tr>
<td>315.839</td>
<td>17370</td>
<td>387.568</td>
<td>204254</td>
</tr>
<tr>
<td>320.056</td>
<td>20841</td>
<td></td>
<td></td>
</tr>
<tr>
<td>324.073</td>
<td>24655</td>
<td>Antione eq. for temp</td>
<td></td>
</tr>
<tr>
<td>330.275</td>
<td>3162</td>
<td>range 293–363 K</td>
<td></td>
</tr>
<tr>
<td>334.497</td>
<td>37286</td>
<td>log $P = A - B/(C + T/K)$</td>
<td></td>
</tr>
<tr>
<td>339.931</td>
<td>45699</td>
<td>$P$/kPa</td>
<td></td>
</tr>
<tr>
<td>344.142</td>
<td>53227</td>
<td>A</td>
<td>6.1734</td>
</tr>
<tr>
<td>348.439</td>
<td>61895</td>
<td>B</td>
<td>1277.452</td>
</tr>
<tr>
<td>353.84</td>
<td>73237</td>
<td>C</td>
<td>–56.889</td>
</tr>
<tr>
<td>358.929</td>
<td>87873</td>
<td></td>
<td></td>
</tr>
<tr>
<td>362.593</td>
<td>98750</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.3.9.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetrafluorobenzene.
6.1.3.10 Pentafluorobenzene

Common Name: Pentafluorobenzene
Chemical Name: pentafluorobenzene
CAS Registry No: 363-72-4
Molecular Formula: C₆HF₅
Molecular Weight: 168.064
Melting Point (°C):
-47.4 (Lide 2003)
Boiling Point (°C):
85.74 (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
111.0 (20°C, calculated-density, Stephenson & Malanowski 1987)
121.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
32.38 (Ambrose 1968)
Enthalpy of Fusion, ΔHₖ (kJ/mol):
Entropy of Fusion, ΔSₖ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
9015* (24.78°C, static method, measured range 24.78–84.98°C, Patrick & Prosser 1964)
log (P/mmHg) = 6.94904 – 1218.91/(213.313 + t/°C); temp range 24.98–84.98°C, Patrick & Prosser 1964)
log (P/mmHg) = 7.03348 – 1253.043/(215.897 + t/°C); temp range 48.7–94.3°C (Antoine eq. from ebulliometric measurements, Ambrose 1968)
log (P/kPa) = 6.07634 – 1220.72/(213.425 + t/°C); temp range 24.78–84.98°C (Antoine eq. derived from Patrick & Prosser 1946 data, Boublik et al. 1984)
log (P/kPa) = 6.15571 – 1250.946/(−57.457 + T/K); temp range 322–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.20712 – 1282.574/(−53.619 + T/K); temp range 358–397 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.47368 – 1477.401/(−27.81 + T/K); temp range 393–479 K (Antoine eq.-III, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₖ₇₉:
2.53 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₖ₈₉:
Bioconcentration Factor, log BCF or log K₆:
Sorption Partition Coefficient, log Kₐ₆:
Environmental Fate Rate Constants, k and Half-Lives, tₜ:
Half-Lives in the Environment:
TABLE 6.1.3.10.1
Reported vapor pressures of pentafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{(T/K)} \quad (1) \\
\ln P &= A - \frac{B}{(T/K)} \quad (1a) \\
\log P &= A - \frac{B}{(C + t/°C)} \quad (2) \\
\ln P &= A - \frac{B}{(C + t/°C)} \quad (2a) \\
\log P &= A - \frac{B}{(C + T/K)} \quad (3) \\
\log P &= A - \frac{B}{(T/K)} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

Patrick & Prosser 1964

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>(\log P)</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>(\ln P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.78</td>
<td>9015</td>
<td>48.729</td>
<td>48.729</td>
<td>26584</td>
<td></td>
</tr>
<tr>
<td>29.85</td>
<td>11492</td>
<td>54.355</td>
<td>54.355</td>
<td>33360</td>
<td></td>
</tr>
<tr>
<td>34.85</td>
<td>14540</td>
<td>59.041</td>
<td>59.041</td>
<td>40023</td>
<td></td>
</tr>
<tr>
<td>39.85</td>
<td>18206</td>
<td>63.033</td>
<td>63.033</td>
<td>46499</td>
<td></td>
</tr>
<tr>
<td>44.85</td>
<td>22507</td>
<td>66.698</td>
<td>66.698</td>
<td>53178</td>
<td></td>
</tr>
<tr>
<td>49.85</td>
<td>27527</td>
<td>69.91</td>
<td>69.91</td>
<td>59642</td>
<td></td>
</tr>
<tr>
<td>54.87</td>
<td>33877</td>
<td>72.828</td>
<td>72.828</td>
<td>66050</td>
<td></td>
</tr>
<tr>
<td>59.92</td>
<td>41071</td>
<td>75.604</td>
<td>75.604</td>
<td>72643</td>
<td></td>
</tr>
<tr>
<td>64.95</td>
<td>49217</td>
<td>78.158</td>
<td>78.158</td>
<td>79163</td>
<td></td>
</tr>
<tr>
<td>69.95</td>
<td>59052</td>
<td>80.643</td>
<td>80.643</td>
<td>85953</td>
<td></td>
</tr>
<tr>
<td>74.95</td>
<td>70191</td>
<td>82.998</td>
<td>82.998</td>
<td>92792</td>
<td></td>
</tr>
<tr>
<td>79.95</td>
<td>82728</td>
<td>85.123</td>
<td>85.123</td>
<td>99333</td>
<td></td>
</tr>
<tr>
<td>84.98</td>
<td>97125</td>
<td>85.496</td>
<td>85.496</td>
<td>100521</td>
<td></td>
</tr>
</tbody>
</table>

Ambrose 1968

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>(\ln P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>86.3</td>
<td>89.093</td>
<td>112557</td>
</tr>
</tbody>
</table>

Antoine eq. 91.014 119417

eq. 2 P/mmHg

A 6.94904

B 1218.91

C 213.313

\[\Delta H_v/(kJ \text{ mol}^{-1}) = \]

at 25°C 36.67

at bp 32.07

FIGURE 6.1.3.10.1 Logarithm of vapor pressure versus reciprocal temperature for pentafluorobenzene.
6.1.3.11 Hexafluorobenzene

Common Name: Hexafluorobenzene
Synonym: perfluorobenzene
Chemical Name: hexafluorobenzene
CAS Registry No: 392-56-3
Molecular Formula: C\textsubscript{6}F\textsubscript{6}
Molecular Weight 180.054
Melting Point (°C):
\begin{itemize}
  \item 5.0.3 (Lide 2003)
\end{itemize}
Boiling Point (°C):
\begin{itemize}
  \item 80.26 (Lide 2003)
\end{itemize}
Density (g/cm\textsuperscript{3}):
\begin{itemize}
  \item 1.61866, 1.60732 (20°C, 25°C, Riddick et al. 1986)
  \item 1.6184 (20°C, Lide 2003)
\end{itemize}
Molar Volume (cm\textsuperscript{3}/mol):
\begin{itemize}
  \item 115.8 (calculated-density, Stephenson & Malanowski 1987)
  \item 126.0 (calculated-Le Bas method at normal boiling point)
\end{itemize}
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
\begin{itemize}
  \item 35.47 (25°C, Findlay 1969)
  \item 35.69, 31.67 (25°C, bp, Riddick et al. 1986)
\end{itemize}
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):

Fugacity Ratio at 25°C, F:

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
\begin{itemize}
  \item 11196* (24.78°C, static method, measured range 19.75–84.98°C, Patrick & Prosser 1964)
  \item log (P/mmHg) = 7.39075 – 1432.91/(237.470 + t°C); temp range 19.76–84.98°C, Patrick & Prosser 1964)
  \item 19957* (37.303°C, gas saturation/manometer, measured range 37.303–88.79°C, Counsell et al. 1965)
  \item 11402* (25.1°C, Hg manometer, measured range 4.74–47.85°C, Findlay 1969)
  \item log (P/mmHg) = 6.86088 – 1152.442/(208.663 + t°C); temp range 4.74–47.85 (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)
  \item 10733* (24.005°C, ebulliometry, measured range 290–377 K, Ambrose 1981)
  \item log (P/kPa) = 6.05252 – 1177.973/(210.677 + t°C); temp range 19.75–84.98°C (Antoine eq. derived from Patrick & Prosser 1964 data, Boublik et al. 1984)
  \item log (P/kPa) = 6.14363 – 1220.148/(214.610 + t°C); temp range 37.3–88.8°C (Antoine eq. derived from Counsell et al. 1965 data, Boublik et al. 1984)
  \item log (P/kPa) = 6.15011 – 1223.989/(215.084 + t°C); temp range 17–104°C (Antoine eq. derived from Ambrose 1981 data, Boublik et al. 1984)
  \item 10733* (selected, Riddick et al. 1986)
  \item log (P/kPa) = 6.14213 – 1219.41/(214.55 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
  \item log (P/kPa) = 11.49514 – 3518.13/(44.44 + T/K); temp range 215–278 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\end{itemize}
log \( (P_{i}/\text{kPa}) = 6.15233 - 1224.974/(–57.984 + T/\text{K}) \); temp range 278–354 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( (P_{i}/\text{kPa}) = 6.19544 - 1251.177/(–54.775 + T/\text{K}) \); temp range 348–389 K (Antoine eq.-III, Stephenson & Malanowski 1987)

\[
\log (P/\text{mmHg}) = –38.8085 – 1.3422 \times 10^3/(T/\text{K}) + 22.204 \cdot \log (T/\text{K}) – 3.8813 \times 10^{–221} \cdot (T/\text{K})^2;
\]

temp range 278–517 K (vapor pressure eq., Yaws et al. 1994)

Henry’s Law Constant \((\text{Pa} \cdot \text{m}^3/\text{mol} \text{ at } 25^\circ\text{C})\):

Octanol/Water Partition Coefficient, \(\log K_{\text{OW}}\):

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.22</td>
<td>shake flask, Log P Database, Hansch &amp; Leo 1987</td>
</tr>
<tr>
<td>2.22</td>
<td>recommended, Sangster 1993</td>
</tr>
<tr>
<td>2.54</td>
<td>recommended, Hansch et al. 1995</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, \(\log K_{\text{OA}}\):

Bioconcentration Factor, \(\log BCF\) or \(\log K_B\):

Sorption Partition Coefficient, \(\log K_{\text{OC}}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):

Volatilization:

- Photolysis: rate constant \(k = 1.7 \times 10^{-5} \text{ h}^{-1}, 1.32 \times 10^{-4} \text{ h}^{-1}\), with \(\text{H}_2\text{O}_2\) under photolysis at 25°C in F-113 solution and with HO in the gas (Dilling et al. 1988).

- Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO}_3}\) with \(\text{NO}_3\) radical and \(k_{\text{O}_3}\) with \(\text{O}_3\) or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

  - \(k_{\text{OH}} = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

  - \(k_{\text{OH}}(\text{obs}) = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\), and \(k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at room temp. (Atkinson 1985)

  - \(k_{\text{OH}}* = (1.61 \pm 0.24) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

  - \(k_{\text{OH}}* = 1.72 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (recommended, Atkinson 1989)

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>(t/\circ\text{C})</th>
<th>(P/\text{Pa})</th>
<th>(t/\circ\text{C})</th>
<th>(P/\text{Pa})</th>
<th>(t/\circ\text{C})</th>
<th>(P/\text{Pa})</th>
<th>(t/\circ\text{C})</th>
<th>(P/\text{Pa})</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.75</td>
<td>8714</td>
<td>37.303</td>
<td>19957</td>
<td>4.74</td>
<td>3849</td>
<td>290.029</td>
<td>7747</td>
</tr>
<tr>
<td>24.78</td>
<td>11196</td>
<td>43.536</td>
<td>26124</td>
<td>5.7</td>
<td>4065</td>
<td>293.503</td>
<td>8940</td>
</tr>
<tr>
<td>29.85</td>
<td>14289</td>
<td>49.109</td>
<td>32880</td>
<td>7.07</td>
<td>4426</td>
<td>297.155</td>
<td>10733</td>
</tr>
<tr>
<td>34.85</td>
<td>17966</td>
<td>53.82</td>
<td>39638</td>
<td>7.14</td>
<td>4429</td>
<td>300.564</td>
<td>12667</td>
</tr>
<tr>
<td>39.85</td>
<td>22461</td>
<td>57.848</td>
<td>46271</td>
<td>9.77</td>
<td>5118</td>
<td>304.801</td>
<td>15466</td>
</tr>
<tr>
<td>44.85</td>
<td>27687</td>
<td>61.585</td>
<td>53199</td>
<td>17.23</td>
<td>7646</td>
<td>309.383</td>
<td>19.045</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
### TABLE 6.1.3.11.1 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Method</td>
<td>static method-Hg manometer</td>
<td>gas saturation/manometer</td>
<td>Hg manometer</td>
<td>comparative ebulliometry</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
<td>T/K</td>
</tr>
<tr>
<td>49.85</td>
<td>33860</td>
<td>64.655</td>
<td>59496</td>
<td>17.23</td>
</tr>
<tr>
<td>54.87</td>
<td>41446</td>
<td>67.63</td>
<td>66152</td>
<td>19.68</td>
</tr>
<tr>
<td>59.92</td>
<td>50169</td>
<td>70.172</td>
<td>72295</td>
<td>24.28</td>
</tr>
<tr>
<td>64.95</td>
<td>59860</td>
<td>72.666</td>
<td>78764</td>
<td>24.4</td>
</tr>
<tr>
<td>69.95</td>
<td>71569</td>
<td>75.337</td>
<td>86190</td>
<td>25.1</td>
</tr>
<tr>
<td>74.95</td>
<td>84741</td>
<td>77.535</td>
<td>92707</td>
<td>27.08</td>
</tr>
<tr>
<td>80.05</td>
<td>100199</td>
<td>79.632</td>
<td>99284</td>
<td>29.92</td>
</tr>
<tr>
<td>84.98</td>
<td>117109</td>
<td>81.446</td>
<td>105264</td>
<td>29.92</td>
</tr>
<tr>
<td>Antoine eq.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 2 P/mmHg</td>
<td>87.027</td>
<td>125463</td>
<td>41.81</td>
<td>24289</td>
</tr>
<tr>
<td>A</td>
<td>7.39075</td>
<td>88.79</td>
<td>132447</td>
<td>47.32</td>
</tr>
<tr>
<td>B</td>
<td>1432, 91</td>
<td>47.85</td>
<td>31064</td>
<td>358.125</td>
</tr>
<tr>
<td>C</td>
<td>237.470</td>
<td>bp/°C</td>
<td>80.261</td>
<td>362.14</td>
</tr>
<tr>
<td>Antoine eq.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 2 P/mmHg</td>
<td>80.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>∆Hv/(kJ mol⁻¹) =</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>35.75</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>at bp</td>
<td>32.70</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 6.1.3.11.1** Logarithm of vapor pressure versus reciprocal temperature for hexafluorobenzene.

© 2006 by Taylor & Francis Group, LLC
6.1.3.12 Pentafluorotoluene

Common Name: Pentafluorotoluene
Synonym: 2, 3, 4, 5, 6-pentafluorotoluene
Chemical Name: 2, 3, 4, 5, 6-pentafluorotoluene
CAS Registry No: 771-56-2
Molecular Formula: C\(_7\)H\(_3\)F\(_5\), C\(_6\)(CH\(_3\))F\(_5\)
Molecular Weight: 182.091
Melting Point (°C):
-29.78 (Lide 2003)
Boiling Point (°C):
117.5 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
1.440 (Lide 2003)
Molar Volume (cm\(^3\)/mol):
126.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
143.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_V\) (kJ/mol):
35.19 (Ambrose 1968)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5056* (39.164°C, ebulliometry, measured range 39–138°C or pressure range 30–1500 mmHg, Ambrose 1968)
\[\log (P/\text{mmHg}) = 7.07209 - 1384.062/(212.731 + t/°C); \text{ temp range ~76–127°C or pressure range 200–1000 mmHg}\]
\[\log (P/\text{mmHg}) = 7.09119 - 1388.288/(213.646 + t/°C); \text{ temp range 39–138°C or pressure range 30–1500 mmHg}\]
\[\log (P/\text{mmHg}) = 13.68523 - 2813.814/(T/K) - 1.2691 \times 10^{-5}(T/K)^2 + 0.8888 \times 10^{-5}(T/K)^3; \text{ temp range 39–138°C}\]
\[\log (P_p/kPa) = 6.19445 - 1382.934/(– 60.494 + T/K); \text{ temp range 312–416 K (Antoine eq.-I, Stephenson & Malanowski 1987)}\]
\[\log (P_p/kPa) = 6.21241 - 1394.345/(– 59.194 + T/K); \text{ temp range 348–401 K (Antoine eq.-II, Stephenson & Malanowski 1987)}\]
Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):
Octanol/Water Partition Coefficient, log \(K_{OW}\):
Octanol/Air Partition Coefficient, log \(K_{OA}\):
Bioconcentration Factor, log \(BCF\) or log \(K_B\):
Sorption Partition Coefficient, log \(K_{OC}\):
Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):
Half-Lives in the Environment:
TABLE 6.1.3.12.1
Reported vapor pressures of pentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations

| \( \log P = A - B/(T/K) \) | \( \ln P = A - B/(T/K) \) |
| \( \log P = A - B/(C + t/°C) \) | \( \ln P = A - B/(C + t/°C) \) |
| \( \log P = A - B/(C + T/K) \) |
| \( \log P = A - B/(T/K) - C \cdot \log (T/K) \) |
| \( \log P = A - B/(T/K) - C \cdot (T/K)^2 \) |

Ambrose 1968

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( \text{eq.} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>39.164</td>
<td>5056</td>
<td>Antoine eq.</td>
</tr>
<tr>
<td>50.578</td>
<td>8787</td>
<td>eq. 2 P/mmHg</td>
</tr>
<tr>
<td>58.357</td>
<td>12354</td>
<td>A 7.09119</td>
</tr>
<tr>
<td>62.734</td>
<td>14885</td>
<td>B 1396.198</td>
</tr>
<tr>
<td>66.375</td>
<td>17308</td>
<td>C 214.112</td>
</tr>
<tr>
<td>72.174</td>
<td>21831</td>
<td>for full range 30–1000 mmHg</td>
</tr>
<tr>
<td>76.551</td>
<td>25854</td>
<td>or temp range 39–138°C</td>
</tr>
<tr>
<td>81.824</td>
<td>31492</td>
<td></td>
</tr>
<tr>
<td>85.651</td>
<td>36176</td>
<td>eq. 2 P/mmHg</td>
</tr>
<tr>
<td>92.625</td>
<td>46172</td>
<td>A 7.07209</td>
</tr>
<tr>
<td>97.287</td>
<td>54019</td>
<td>B 1384.062</td>
</tr>
<tr>
<td>102.370</td>
<td>63757</td>
<td>C 212.731</td>
</tr>
<tr>
<td>107.382</td>
<td>66700</td>
<td>for range 200–1000 mmHg</td>
</tr>
<tr>
<td>112.608</td>
<td>87655</td>
<td>or temp range ~76–127°C</td>
</tr>
<tr>
<td>116.158</td>
<td>97433</td>
<td></td>
</tr>
<tr>
<td>117.884</td>
<td>102509</td>
<td>Cragoe eq.</td>
</tr>
<tr>
<td>118.979</td>
<td>105812</td>
<td>eq. 5 P/mmHg</td>
</tr>
<tr>
<td>123.337</td>
<td>119831</td>
<td>A 13.68523</td>
</tr>
<tr>
<td>127.924</td>
<td>136155</td>
<td>B 2813.814</td>
</tr>
<tr>
<td>133.176</td>
<td>156948</td>
<td>C 1.2691 \times 10^{-2}</td>
</tr>
<tr>
<td>138.226</td>
<td>179191</td>
<td>D 0.8888 \times 10^{-5}</td>
</tr>
</tbody>
</table>

bp/°C 117.493

\( \Delta H_v = 35.18 \text{ kJ mol}^{-1} \)
6.1.3.13 Chloropentafluorobenzene

Common Name: Chloropentafluorobenzene
Synonym: 
Chemical Name: chloropentafluorobenzene
CAS Registry No: 344-07-0
Molecular Formula: C₆ClF₅
Molecular Weight: 202.509
Melting Point (°C):
117.96 \(\text{Lide 2003}\)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
129.2 \(\text{calculated-density, Stephenson & Malanowski 1987}\)
141.9 \(\text{calculated-Le Bas method at normal boiling point}\)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
35.15 \(\text{Ambrose 1968}\)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4186* \(\text{(35.576°C, ebulliometry, measured range 36–144°C or pressure range 30–1500 mmHg, Ambrose 1968)}\)
\(\log (P/\text{mmHg}) = 7.06976 – 1389.841/(213.833 + t/°C)}\); temp range ~80–127°C or pressure range 100–1000 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
\(\log (P/\text{mmHg}) = 7.06747 – 1388.288/(213.646 + t/°C)}\); temp range 36–144°C or pressure range 30–1500 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)
\(\log (P/\text{mmHg}) = 14.36999 – 2894.645/(T/K) – 1.4603 \times 10^{-2}(T/K) + 1.0612 \times 10^{-5}(T/K)^2\); temp range 36–144°C (Cragoe eq., ebulliometry, Ambrose 1968)
\(\log (P/\text{mmHg}) = 14.36999 – 2894.645/(T/K) – 1.4603 \times 10^{-2}(T/K) + 1.0612 \times 10^{-5}(T/K)^2\); temp range 348–402 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\(\log (P/\text{mmHg}) = 14.36999 – 2894.645/(T/K) – 1.4603 \times 10^{-2}(T/K) + 1.0612 \times 10^{-5}(T/K)^2\); temp range 307–417 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, \(\log K_{ow}\):
Octanol/Air Partition Coefficient, \(\log K_{oa}\):
Bioconcentration Factor, \(\log BCF\) or \(\log K_b\):
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 6.1.3.13.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of chloropentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

$$
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\cdot\log(T/K) \quad (4) \\
\log P &= A - B/(T/K) - C\cdot(T/K)^2 \quad (5)
\end{align*}

Ambrose 1968

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.576</td>
<td>4186</td>
</tr>
<tr>
<td>44.790</td>
<td>6614</td>
</tr>
<tr>
<td>55.927</td>
<td>11028</td>
</tr>
<tr>
<td>61.852</td>
<td>14216</td>
</tr>
<tr>
<td>65.865</td>
<td>16811</td>
</tr>
<tr>
<td>70.085</td>
<td>19929</td>
</tr>
<tr>
<td>75.343</td>
<td>24459</td>
</tr>
<tr>
<td>81.691</td>
<td>31024</td>
</tr>
<tr>
<td>86.763</td>
<td>37244</td>
</tr>
<tr>
<td>92.135</td>
<td>44900</td>
</tr>
<tr>
<td>97.254</td>
<td>53331</td>
</tr>
<tr>
<td>102.357</td>
<td>62963</td>
</tr>
<tr>
<td>107.155</td>
<td>73251</td>
</tr>
<tr>
<td>112.764</td>
<td>86927</td>
</tr>
<tr>
<td>116.436</td>
<td>96926</td>
</tr>
<tr>
<td>117.448</td>
<td>99832</td>
</tr>
<tr>
<td>118.893</td>
<td>104118</td>
</tr>
<tr>
<td>125.580</td>
<td>118997</td>
</tr>
<tr>
<td>127.992</td>
<td>134517</td>
</tr>
<tr>
<td>133.467</td>
<td>155905</td>
</tr>
<tr>
<td>138.689</td>
<td>178705</td>
</tr>
<tr>
<td>144.131</td>
<td>205189</td>
</tr>
</tbody>
</table>

bp/°C 117.954
$\Delta H_v = 35.15 \text{ kJ mol}^{-1}$
6.1.3.14  Pentafluorophenol

Common Name: Pentafluorophenol
Synonym: pentafluorophenol
Chemical Name: pentafluorophenol
CAS Registry No: 771-61-9
Molecular Formula: C₆(OH)F₅
Molecular Weight: 184.063
Melting Point (°C):
37.5  (Lide 2003)
Boiling Point (°C):
145.6  (Lide 2003)
Density (g/cm³):

Molar Volume (cm³/mol):
128.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
41.59  (Ambrose 1968)
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.754 (mp at 37.5°C)
Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
26578*  (105.448°C, ebulliometry, measured range 105.5–155°C, Ambrose 1968)
log (P/mmHg) = 7.06296 – 1377.185/(183.680 + t°C); temp range 105–155°C (Antoine eq. from ebulliometric measurements, Ambrose 1968)
log (P/kPa) = 11.291 – 3523/(T/K); temp range 273–296 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.18665 – 1377.011/(– 89.435 + T/K); temp range 378–428 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log $K_{ow}$:
3.23  (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$:
Bioconcentration Factor, log BCF or log $K_{bi}$:
Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:
### TABLE 6.1.3.14.1
Reported vapor pressures of pentafluorophenol at various temperatures
Ambrose 1968

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/\text{Pa} )</th>
<th>( t/°C )</th>
<th>( P/\text{Pa} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>105.448</td>
<td>26578</td>
<td>153.041</td>
<td>125269</td>
</tr>
<tr>
<td>111.328</td>
<td>32076</td>
<td>154.963</td>
<td>132153</td>
</tr>
<tr>
<td>116.192</td>
<td>39393</td>
<td></td>
<td></td>
</tr>
<tr>
<td>120.720</td>
<td>46087</td>
<td>bp/°C</td>
<td>145.621</td>
</tr>
<tr>
<td>124.827</td>
<td>52940</td>
<td>( \Delta H_v = 41.59 \text{ kJ mol}^{-1} )</td>
<td></td>
</tr>
<tr>
<td>128.292</td>
<td>59367</td>
<td>Antoine eq.</td>
<td></td>
</tr>
<tr>
<td>131.565</td>
<td>65904</td>
<td>log ( P = A - \frac{B}{C + t/°C} )</td>
<td></td>
</tr>
<tr>
<td>134.647</td>
<td>72670</td>
<td>P/mmHg</td>
<td></td>
</tr>
<tr>
<td>137.240</td>
<td>78804</td>
<td>A</td>
<td>7.03488</td>
</tr>
<tr>
<td>140.302</td>
<td>86489</td>
<td>B</td>
<td>1253.043</td>
</tr>
<tr>
<td>142.507</td>
<td>92412</td>
<td>C</td>
<td>215.897</td>
</tr>
<tr>
<td>145.002</td>
<td>99506</td>
<td>full range 200–1000 mmHg</td>
<td></td>
</tr>
<tr>
<td>147.069</td>
<td>105684</td>
<td>or temp range 105–155°C</td>
<td></td>
</tr>
<tr>
<td>149.090</td>
<td>112009</td>
<td></td>
<td></td>
</tr>
<tr>
<td>151.190</td>
<td>118917</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.1.4 Bromobenzenes and Bromotoluenes

6.1.4.1 Bromobenzene

Common Name: Bromobenzene
Synonym: phenyl bromide
Chemical Name: bromobenzene
CAS Registry No: 108-86-1
Molecular Formula: C\textsubscript{6}H\textsubscript{5}Br
Molecular Weight: 157.008

Melting Point (°C):
-30.72 (Dean 1985; Lide 2003)

Boiling Point (°C):
156.06 (Dreisbach & Martin 1949; Dreisbach 1955; Lide 2003)

Density (g/cm\textsuperscript{3} at 20°C):
1.4950, 1.48824 (20°C, Dreisbach 1955)
1.4950 (Weast 1982–83; Lide 2003)
1.4952 (Dean 1985)

Molar Volume (cm\textsuperscript{3}/mol):
105.0 (20°C, calculated-density, Chiou 1985)
119.3 (Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
10.63 (Dreisbach 1955)
10.70 (Riddick et al. 1986)

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

446 (30°C, shake flask-IR, Gross & Saylor 1931)
410 (shake flask-UV, Andrews & Keefer 1950)
462 (shake flask-interferometry, Donahue & Bartell 1952)
328 (Deno & Berkheimer 1960)
458.5 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
457* (shake flask-spectrophotometry, measured range 10–35°C, Vesala 1973)
446 (shake flask-UV, Vesala 1974)
148* (shake flask-GC, measured range 5–45.5°C, Nelson & Smit 1978)
360 (shake flask-UV, Yalkowsky et al. 1979)
274* (summary of literature data, temp range 25–40°C, Horvath 1982)
411 (generator column-HPLC/UV, Wasik et al. 1983)
330 (headspace-GC, McNally & Grob 1984)
445* (recommended, temp range 10–40°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 1.8293 - 1.35675 \times 10^{-2}(T/K) + 2.99322 \times 10^{-5}(T/K)^2; $ temp range 288–308 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
384* (20°C, limiting activity coeff. by equilibrium air stripping-GC, temp range 10–50°C, Hovorka & Dohnal 1997)
384* (estimated- RP-HPLC-k’ correlation, measured range 5–35°C, Finizio & Di Guardo 2001)
Chlorobenzenes and Other Halogenated Mononuclear Aromatics

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- \( \log (P/\text{mmHg}) = 7.25422 – 1688.4/(230 + t/°C) \) (Antoine eq., Dreisbach & Martin 1949)
- \( \log (P/\text{mmHg}) = 6.91444 – 1474.06/(209.4 + t/°C) \); temp range 60–190°C (Antoine eq. for liquid state, Dreisbach 1955)
- \( \log (P/\text{mmHg}) = 7.7807 – 2105.4/(T/K) \); temp range 49–131°C (Antoine eq., Weast 1972–73)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

- \( K_{\text{AW}} \) or \( C_W/C_A \) (Hine & Mookerjee 1975)
- \( C_W/C_A \) (gas stripping-GC, Mackay & Shiu 1981, 1990)
- \( K_{\text{AW}} \) (recommended, Mackay & Shiu 1981)
- \( K_{\text{AW}} \) (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \) (at 25°C or as indicated):

- \( \log K_{\text{OW}} = 2.99 \) (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
- \( \log K_{\text{OW}} = 3.03 \) (calculated-fragment const.; Rekker 1977)
- \( \log K_{\text{OW}} = 3.16 \) (HPLC-K’ correlation, McDuffie 1981)
- \( \log K_{\text{OW}} = 2.98 \) (generator column-HPLC, Wasik et al. 1983)
- \( \log K_{\text{OW}} = 3.02 \) (HPLC-RT correlation, D’Amboise & Hanai 1982)
- \( \log K_{\text{OW}} = 3.01 \) (shake flask-GC, Watarai et al. 1982)
- \( \log K_{\text{OW}} = 3.02 \) (HPLC-RT correlation, Eadsforth & Moser 1983)
Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals

3.01 (HPLC-RT correlation, Garst & Wilson 1984)
3.15 (HPLC correlation, Eadsforth 1986)
2.99 (recommended, Sangster 1989, 1993)
2.75, 2.94 (shake flask-UV/VIS spec. 25, 60°C; Kramer & Henze 1990)
2.99 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
3.18 (activated sludge, Freitag et al. 1984)
2.28 (algae, Freitag et al. 1984)
1.68 (fish, Freitag et al. 1984)
1.68, 2.28, 3.18 (fish, algae, activated sludge, Halfon & Reggiani 1986)
1.70 (Freitag et al. 1985)
1.899, 1.928 (calculated-K_{calk}, calculated- MCI \chi, Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC}:
2.18 (soil, selected lit., Kenaga & Goring 1980)
2.18 (calculated-S. Kenaga 1980)
2.80 (calculated-MCI \chi, Koch 1983)
2.56 (calculated-MCI. Sabljic 1984)
2.65 (calculated-MCI, Bahnick & Doucette 1988)
2.65 (HPLC-RT correlation, cyanopropy column, Hodson & Williams 1988)
3.37 (activated carbon, Blum et al. 1994)
2.49 (soil, calculated-MCI \chi, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Vaporization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO3 radical and k_{O3} with O3 or as indicated, *data at other temperatures see reference:
k_{OH}^* = 7.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp., measured range 245–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)}
k_{OH}(calc) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(obs) = 0.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1987)}
k_{OH}^* = (9.15 \pm 0.97) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)}
k_{OH} = 7.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ independent of temperature over the range 234–362 K (Atkinson 1989)}
k_{OH}(calc) = 0.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}

Hydrolysis:
Biodegradation: relative rate from activated sludge approximately of 34.8% CO2 (Freitag et al. 1984).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
TABLE 6.1.4.1.1
Reported aqueous solubilities of bromobenzene at various temperatures

\[ S(\text{wt}%) = 1.09002 \times 10^{-2} + 4.43314 \times 10^{-4}(t/°C) + 1.20007 \times 10^{-5}(t/°C)^2 - 1.33342 \times 10^{-7}(t/°C)^3 \]  (1)

\[ S/(\text{g/kg}) = 1.8293 - 1.35675 \times 10^{-2}(T/K) + 2.99322 \times 10^{-5}(T/K)^2 \]  (2)

1. Vesala 1973
   - shake flask-UV
   - summary of literature data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>389.57</td>
</tr>
<tr>
<td>15.2</td>
<td>406.05</td>
</tr>
<tr>
<td>19.6</td>
<td>411.07</td>
</tr>
<tr>
<td>25.0</td>
<td>457.19</td>
</tr>
<tr>
<td>30.0</td>
<td>464.56</td>
</tr>
<tr>
<td>35.0</td>
<td>489.19</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>387</td>
</tr>
<tr>
<td>15</td>
<td>405</td>
</tr>
<tr>
<td>20</td>
<td>424</td>
</tr>
<tr>
<td>25</td>
<td>445</td>
</tr>
<tr>
<td>30</td>
<td>467</td>
</tr>
<tr>
<td>35</td>
<td>491</td>
</tr>
<tr>
<td>40</td>
<td>516</td>
</tr>
</tbody>
</table>

2. Hovorka & Dohnal 1997
   - γ∞ by air stripping-GC

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>354.6</td>
</tr>
<tr>
<td>20</td>
<td>384.3</td>
</tr>
<tr>
<td>30</td>
<td>427.6</td>
</tr>
<tr>
<td>40</td>
<td>499.0</td>
</tr>
<tr>
<td>50</td>
<td>598.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>278</td>
</tr>
<tr>
<td>15</td>
<td>274.5</td>
</tr>
<tr>
<td>25</td>
<td>384</td>
</tr>
<tr>
<td>35</td>
<td>368</td>
</tr>
</tbody>
</table>

\[ \ln x \] versus 1/T

**FIGURE 6.1.4.1.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromobenzene.
## TABLE 6.1.4.1.2
Reported vapor pressures of bromobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th></th>
<th>Kahlbaum 1898 static method*</th>
<th>Stull 1947 summary of lit. data</th>
<th>Dreisbach &amp; Shrader 1949 ebulliometry</th>
<th>Dreyer et al. 1954</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>29.8</td>
<td>666.6</td>
<td>2.9</td>
<td>133.3</td>
<td>71.86</td>
</tr>
<tr>
<td>40.6</td>
<td>1333.2</td>
<td>27.8</td>
<td>666.6</td>
<td>76.39</td>
</tr>
<tr>
<td>47.7</td>
<td>1999.8</td>
<td>40</td>
<td>1333</td>
<td>80.08</td>
</tr>
<tr>
<td>52.8</td>
<td>2666.4</td>
<td>53.8</td>
<td>2666</td>
<td>83.99</td>
</tr>
<tr>
<td>57.3</td>
<td>3333</td>
<td>68.6</td>
<td>5333</td>
<td>96.32</td>
</tr>
<tr>
<td>61.2</td>
<td>3999.7</td>
<td>78.1</td>
<td>7999</td>
<td>127.47</td>
</tr>
<tr>
<td>67.7</td>
<td>4666</td>
<td>90.8</td>
<td>13332</td>
<td>140.69</td>
</tr>
<tr>
<td>70.4</td>
<td>5333</td>
<td>110.1</td>
<td>26664</td>
<td>158.06</td>
</tr>
<tr>
<td>73.0</td>
<td>6666.1</td>
<td>132.3</td>
<td>53329</td>
<td>90.82</td>
</tr>
<tr>
<td>82.8</td>
<td>9999.2</td>
<td>156.2</td>
<td>101325</td>
<td></td>
</tr>
<tr>
<td>90.0</td>
<td>13332</td>
<td></td>
<td>mp/°C</td>
<td></td>
</tr>
<tr>
<td>109.5</td>
<td>26664</td>
<td></td>
<td>–30.7</td>
<td></td>
</tr>
<tr>
<td>122.0</td>
<td>39997</td>
<td></td>
<td></td>
<td>eq. 2</td>
</tr>
<tr>
<td>131.6</td>
<td>53329</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>139.4</td>
<td>66661</td>
<td></td>
<td></td>
<td>A</td>
</tr>
<tr>
<td>145.9</td>
<td>79993</td>
<td></td>
<td></td>
<td>B</td>
</tr>
<tr>
<td>152.5</td>
<td>93326</td>
<td></td>
<td></td>
<td>C</td>
</tr>
<tr>
<td>155.5</td>
<td>101325</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*complete list see ref.

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
FIGURE 6.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for bromobenzene.
6.1.4.2 1,2-Dibromobenzene

Common Name: 1,2-Dibromobenzene
Synonym: o-dibromobenzene
Chemical Name: 1,2-Dibromobenzene
CAS Registry No: 583-53-9
Molecular Formula: C₆H₄Br₂
Molecular Weight: 235.904
Melting Point (°C):
7.1 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
225 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.98429, 1.9767 (20°C, 25°C, Dreisbach 1955)
1.9843 (20°C, Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
120.2 (calculated-density, Stephenson & Malanowski 1987)
142.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
59.31, 42.594 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH₉₅ (kJ/mol):
7.279 (Dreisbach 1955)
Entropy of Fusion, ΔS₉₅ (J/mol K):
Water Solubility (g/m³ or mg/L at 25°C):
74.55 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
74.8 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/㎜Hg) = 7.44451 – 2050.3/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
25.7 (calculated by formula, Dreisbach 1955)
log (P/㎜Hg) = 7.10265 – 1825.77/(207.0 + t°C); temp range 115–295°C (Antoine eq. for liquid state, Dreisbach 1955)
26.0 (interpolated-Antoine eq., Dean 1985, 1992)
log (P/㎜Hg) = 7.50128 – 2093.1/(t°C + 230); temp range 28–117°C (Antoine eq., Dean 1985, 1992)
log (P/㎜Hg) = 7.10265 – 1825.77/(t°C + 207); temp range 117–300°C (Antoine eq., Dean 1985, 1992)
22.80 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.22755 – 1825.77/(T/K – 66.15); temp range 388–588 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
3.64 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)
3.68 (HPLC-RT correlation, Garst & Wilson 1984)
3.64 (recommended, Sangster 1993)
3.64 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:

2.70; 3.50  \( (\text{Pimephales promelas; Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996}) \)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{\frac{1}{2}} \):

Half-Lives in the Environment:
6.1.4.3 1,3-Dibromobenzene

Common Name: 1,3-Dibromobenzene
Synonym: m-dibromobenzene
Chemical Name: 1,3-Dibromobenzene
CAS Registry No: 108-36-1
Molecular Formula: C₆H₄Br₂
Molecular Weight: 235.904
Melting Point (°C):

-7.0 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

218 (Lide 2003)

Density (g/cm³ at 20°C):

1.9523 (20°C, Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):

120.8 (20°C, calculated-density, Stephenson & Malanowski 1987)
142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):

Enthalpy of Fusion, ΔHfus (kJ/mol):

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

67.4 (30°C, shake flask-UV, Hine et al. 1963)
98.45 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
64.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

57.06 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
22.78 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 5.971 – 1603.4/(T/K – 87.55); temp range 417–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

157, 61.05 (calculated-ΔSv, mp and bp, Antoine eq., Yalkowsky & Mishra 1990, Mishra & Yalkowsky 1991)

log (P/mmHg) = 59.2974 – 4.6960 × 10³/(T/K) – 18.444-log (T/K) + 6.7598 × 10–³·(T/K) – 2.5567 × 10–1³·(T/K)²; temp range 226–761 K (vapor pressure eq., Yaw et al. 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kow:

3.75 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)
3.79 (shake flask-GC, Watarai et al. 1982)
3.78 (Oliver & Niimi 1984)
3.74 (HPLC-k’ correlation, Haky & Yeung 1984)
3.75 (recommended, Sangster 1993)
3.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Koa:

Bioconcentration Factor, log BCF:

2.78 (mean value, rainbow trout, Oliver & Niimi 1984)
2.82 (rainbow trout, Oliver 1987)
2.82 (Oncorhynchus mykiss, under flow-through conditions, quoted, Devillers et al. 1996)
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: pseudo-first order reaction rate constant for direct photolysis $k = 0.009$ min$^{-1}$ with $t_{1/2} = 76.8$ min. in dilute aqueous solution (Peijnenburg et al. 1992).

Half-Lives in the Environment:

Air:

Surface water: pseudo-first order reaction rate constant for direct photolysis $k = 0.009$ min$^{-1}$ with $t_{1/2} = 76.8$ min. in dilute aqueous solution (Peijnenburg et al. 1992).

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 3$ d (guppy, Niimi 1987)
6.1.4.4 1,4-Dibromobenzene

Common Name: 1,4-Dibromobenzene
Synonym: \( p \)-dibromobenzene
Chemical Name: 1,4-Dibromobenzene
CAS Registry No: 106-37-6
Molecular Formula: \( \text{C}_6\text{H}_4\text{Br}_2 \)
Molecular Weight: 235.904

Melting Point (°C): 87.43 (Lide 2003)
Boiling Point (°C): 218.5 (Lide 2003)
Density (g/cm³ at 20°C): 1.5742 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
121 (calculated-density, Lande & Banerjee 1981)
142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
4.837 (Ruelle & Kesselring 1997)

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), F: 0.244 (mp at 87.43°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
20.0 (shake flask-UV, Andrews & Keefer 1950)
26.42 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
20.08 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
20.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)
17.0* (shake flask-HPLC, measured range 10–35°C, Kuramochi et al. 2004)

ln \( [S/(mol/L)] = \frac{3151.3.7}{T/K} + 1.06; \) temp range 10–35°C (shake flask-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (61°C, summary of literature data, Stull 1947)
log \( (P/mmHg) = 7.44830 – 2057.2/(230 + t°C) \) (Antoine eq., Dreisbach & Martin 1949)
9.33* (25.8°C, manometer, temp range 25.8–80.5°C, Walsh & Smith 1961)

log \( (P/mmHg) = 11.592 –3826.2/(T/K); \) temp range 25.8–80.5°C (manometer, Walsh & Smith 1961)
17.87 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)

log \( (P/mmHg) = [-0.2185 \times 13047.8/(T/K)] + 8.769771; \) temp range 61–218.6°C (Antoine eq., Weast 1972–73)

3.96* (18.13°C, capacitance manometer; De Kruijff et al. 1981)
7.65 (interpolated, Antoine eq., Stephenson & Malanoski 1987)

log \( P/kPa = 10.717 – 3826.2/(T/K); \) temp range 298–354 K (Antoine eq., solid, Stephenson & Malanoski 1987)
log \( P/kPa = 6.5732 – 2047.2/(T/K – 43.15); \) temp range 373–493 K (Antoine eq., liquid, Stephenson & Malano-

35.95, 53.18 (calculated-bp, Antoine eq., Yalkowsky & Mishra 1990)

Henry’s Law Constant (Pa·m³/mol at 25°C):
106 (derived from \( \gamma_{\infty} \) infinite dilution activity coefficient, Kuramochi et al. 2004)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 3.75 (shake flask, Hansch & Leo 1979)
- 4.07 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
- 4.13 (calculated-fragment const., Yalkowsky et al. 1983)
- 3.79 (shake flask-GC, Watarai et al. 1982)
- 3.89 (Gobas et al. 1989)
- 3.79 (recommended, Sangster 1993)
- 3.79 (recommended, Hansch et al. 1995)
- 3.62 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C:
- 5.21 (calculated-$S_{oct}$ and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
- 3.15 (guppy, lipid-weight based, Gobas et al. 1989)
- 1.96 ($Poecilia reticulata$, under flow-through conditions, Devillers et al. 1996)
- 2.70; 3.40 ($Poecilia reticulata$; $Pimephales promelas$, under static and semi-static conditions, Devillers et al. 1996)
- 3.15 (Gobas et al. 1989)

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\nu$:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $\log k_1 = 2.11\ d^{-1}$; $\log k_2 = 0.15\ d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 6.1.4.4.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities and vapor pressures of 1,4-dibromobenzene at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
<tr>
<td>(Continued)</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
### TABLE 6.1.4.4.1 (Continued)

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kuramochi et al. 2004</td>
<td>Stull 1947 summary of literature data</td>
</tr>
<tr>
<td>shake flask-GC</td>
<td>manometry</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t°C</th>
<th>S/(g m⁻³)</th>
<th>t°C</th>
<th>P/Pa</th>
<th>t°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>ln S = -3151.3/(T/K) + 1.06</td>
<td>mp°C</td>
<td>56.4</td>
<td>129.3</td>
<td>A</td>
<td>13.86395</td>
</tr>
<tr>
<td>S in mol/L</td>
<td>87.5</td>
<td>57.2</td>
<td>136.0</td>
<td>B</td>
<td>3864.8</td>
</tr>
<tr>
<td>57.3</td>
<td>141.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>64.3</td>
<td>238.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>71.8</td>
<td>420.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80.5</td>
<td>791.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp°C</td>
<td>87.24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1 P/mmHg</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>11.592</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3826.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 73.26 \]

### FIGURE 6.1.4.4.1

Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,4-dibromobenzene.
6.1.4.5 1,2,3-Tribromobenzene

Common Name: 1,2,3-Tribromobenzene
Synonym:
Chemical Name: 1,2,3-tribromobenzene
CAS Registry No: 608-21-9
Molecular Formula: C₆H₃Br₃
Molecular Weight: 314.800
Melting Point (°C):
  87.8 (Weast 1982–83)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  137.7 (Ruelle & Kesselring 1997)
  118 (calculated-density, Wang et al. 1992)
  165.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
Enthalpy of Fusion, ∆Hₚ (kJ/mol):
Entropy of Fusion, ∆Sₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₚ = 56 J/mol K), F: 0.242 (mp at 87.8°C)
Water Solubility (g/m³ or mg/L at 25°C):
  2.94 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₗv:
  4.98; 4.25 (quoted exptl value; calculated-molar volume, Wang et al. 1992)
  4.57; 4.42 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Kₗa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₗc:
Environmental Fate Rate Constants, k, or Half-Lives, tₜₕ:
6.1.4.6 1,2,4-Tribromobenzene

Common Name: 1,2,4-Tribromobenzene
Synonym:
Chemical Name: 1,2,4-tribromobenzene
CAS Registry No: 615-54-3
Molecular Formula: C₆H₃Br₃
Molecular Weight: 314.800

Melting Point (°C):
44.5 (Weast 1982–83; Lide 2003)

Boiling Point (°C):
275 (Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
137.7 (Ruelle & Kesselring 1997)
165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):

Enthalpy of Fusion, ΔHₕₚₚ (kJ/mol):

Entropy of Fusion, ΔSₕₚₚ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSₕₚₚ = 56 J/mol K), F: 0.644 (mp at 44.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
9.96 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
10.1 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)
3.67, 7.21, 11.0 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
ln [S/(mol/L)] = –3836.9/(T/K) + 2.19; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C):
31.9 (derived from γ₀W, infinite dilution activity coefficient, Kuramochi et al. 2004)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kₐₜₜ:
4.51 (shake flask-GC, Watarai et al. 1982)
4.54 (Oliver & Niimi 1984)
4.32 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log Kₐₐ:

Bioconcentration Factor, log BCF:
3.63 (rainbow trout, Oliver 1984, Oliver & Niimi 1984, Oliver 1987)

Sorption Partition Coefficient, log Kₐₜ:

Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:

Half-Lives in the Environment:
Biota: t₁/₂ = 3 d in guppy (for tribromobenzenes, Niimi 1987)
6.1.4.7 1,3,5-Tribromobenzene

Common Name: 1,3,5-Tribromobenzene
Synonym:
Chemical Name: 1,3,5-tribromobenzene
CAS Registry No: 626-39-1
Molecular Formula: C₆H₃Br₃
Molecular Weight: 314.800
Melting Point (°C):
  122.8  (Lide 2003)
Boiling Point (°C):
  271  (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  137.7  (Ruelle & Kesselring 1997)
  165.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Fusion, ΔH₆ fus (kJ/mol):
Entropy of Fusion, ΔS₆ fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₆ fus = 56 J/mol K), F: 0.11 (mp at 122.8°C)
Water Solubility (g/m³ or mg/L at 25°C):
  200  (shake flask-residue volume method, Booth & Everson 1948)
  0.04  (Stephen & Stephen 1963)
  0.787  (shake flask-UV, Yalkowsky et al. 1979)
  0.789  (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)
Vapor Pressure (Pa at 25°C):
  5.187  (GC-RT correlation, Watanabe & Tatsukawa 1989)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐw:
  4.51  (shake flask-GC, Watarai et al. 1982)
  5.07  (calculated-fragment const., Yalkowsky et al. 1983)
  4.60, 4.63  (HPLC-RT correlation, Garst 1984)
  5.26  (HPLC-RT correlation, Gobas et al. 1989)
  5.18  (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  4.51  (recommended, Sangster 1993)
  4.51  (selected, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₐa:
Bioconcentration Factor, log BCF:
  3.70  (rainbow trout, Oliver & Niimi 1984, Oliver 1987)
  3.26–4.08 mean 3.97; 3.53–4.20 mean 4.08 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
  4.42  (guppy, lipid-weight based, Gobas et al. 1989)
  3.23; 3.70, 3.97, 4.08 (Poecilia reticulata; Oncorhynchus mykiss, quoted values, Devillers et al. 1996)
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- **Volatileization:**
  - Photolysis: pseudo-first order reaction rate constant in dilute aqueous solution $k = 0.005$ min$^{-1}$ with $t_{1/2} = 140.5$ min. (Peijeneburg et al. 1992).

- **Oxidation:**

- **Hydrolysis:**

- **Biodegradation:**

- **Biotransformation:**
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
    - $\log k_1 = 2.85$ d$^{-1}$; $\log k_2 = -0.38$ d$^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

- **Air:**
  - Surface water: pseudo-first order reaction rate constant for direct photolysis in dilute aqueous solution $k = 0.005$ min$^{-1}$ with $t_{1/2} = 140.5$ min. (Peijeneburg et al. 1992).

- **Groundwater:**

- **Sediment:**

- **Soil:**

- **Biota:** elimination $t_{1/2} = 3$ d (guppy, for tribromobenzenes, Niimi 1987)
6.1.4.8 1,2,4,5-Tetrabromobenzene

![Chemical structure of 1,2,4,5-Tetrabromobenzene]

- **Common Name**: 1,2,4,5-Tetrabromobenzene
- **Synonym**: 1,2,4,5-tetrabromobenzene
- **Chemical Name**: 1,2,4,5-tetrabromobenzene
- **CAS Registry No**: 636-28-2
- **Molecular Formula**: C₆H₂Br₄
- **Molecular Weight**: 393.696
- **Melting Point (°C)**: 182 (Weast 1982–83; Lide 2003)
- **Boiling Point (°C)**: 307.2 (Weast 1982–83)
- **Density (g/cm³ at 20°C)**: 128.2 (calculated-density, Wang et al. 1992)
  - 153.8 (Ruelle & Kesselring 1997)
  - 189.2 (calculated-Le Bas method at normal boiling point)
- **Molar Volume (cm³/mol)**:
  - 128.2 (calculated-density, Wang et al. 1992)
  - 153.8 (Ruelle & Kesselring 1997)
  - 189.2 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Vaporization, ΔHV (kJ/mol)**: 
- **Enthalpy of Fusion, ΔHₜₚ (kJ/mol)**: 
- **Entropy of Fusion, ΔSₜₚ (J/mol K)**: 
- **Fugacity Ratio at 25°C (assuming ΔSₜₚ = 56 J/mol K), F**: 0.0288 (mp at 182°C)
- **Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations)**:
  - 0.0433 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
  - 0.0434 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)
  - 0.044 (shake flask-GC, Kim & Saleh 1990)
  - 0.0182, 0.0435, 0.0778 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
  - ln [S/(mol/L)] = –4967.5/(T/K) + 0.681; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)
- **Vapor Pressure (Pa at 25°C)**: 0.157 (GC-RT correlation, Watanabe & Tatsukawa 1989)
- **Henry’s Law Constant (Pa⋅m³/mol at 25°C)**: 376 (derived from γₗₚ, infinite dilution activity coefficient, Kuramochi et al. 2004)
- **Octanol/Water Partition Coefficient, log Kₜₖₔ**:
  - 5.13 (shake flask-GC, Watarai et al. 1982)
  - 5.25 (HPLC-RT correlation, Garst 1984)
  - 5.56 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  - 5.13 (recommended, Sangster 1993)
  - 5.13 (recommended, Hansch et al. 1995)
  - 5.00 (GC-RT correlation, Kuramochi et al. 2004)
- **Octanol/Air Partition Coefficient, log Kₒₐ**:
- **Bioconcentration Factor, log BCF**:
  - 3.80 (rainbow trout, Banerjee et al. 1980)
  - 2.94–3.68 mean 3.57; 3.40–3.91 mean 3.81 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
3.80 \ (Nendza 1993; quoted, Lu et al. 1999)
3.57 \ (Oncorhynchus mykiss, flow through conditions, Devillers et al. 1996)

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{\frac{1}{2}}$:

Half-Lives in the Environment:

- Biota: $t_{\frac{1}{2}} = 4$ d in guppy (for tetrabromobenzenes, Niimi 1987)
6.1.4.9 Hexabromobenzene

Common Name: Hexabromobenzene
Chemical Name: hexabromobenzene
CAS Registry No: 87-82-1
Molecular Formula: C₆Br₆
Molecular Weight: 551.488

Melting Point (°C):
327 (Weast 1982–83; Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
186 (Ruelle & Kesselring 1997)
235.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):
85 (Tittlemier et al. 2002)

Enthalpy of Fusion, ∆Hfus (kJ/mol):

Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.0011 (mp at 327°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and the reported temperature dependence equations):
0.00016 (22°C, generator column-GC, Opperhuizen 1986)
0.0030 (generator column-GC/ECD, Tittlemier et al. 2002)
0.0000472, 0.00011, 0.000232 (10, 25, 35°C, generator column-HPLC, Kuramochi et al. 2004)
ln [S/(mol/L)] = – 5484.7/(T/K) – 3.85; temp range 10–35°C (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
3.133 × 10⁻⁴ (estimated, Lyman et al. 1982)
3.845 × 10⁻⁴ (GC-RT correlation, Watanabe & Tatsukawa 1989)
7.50 × 10⁻⁴ (supercooled liquid P.L, GC-RT correlation, Tittlemier et al. 2002)
log (P₂/Pa) = – 4454/(T/K) + 11.82 (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.284 (calculated, Meylan & Howard 1991)
0.14 (calculated-P₂/P₁, Tittlemier et al. 2002)
10.8 (derived from γW, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log Kow:
6.15, 6.07 (HPLC-RT correlation, Garst 1984)
7.80 (HPLC-RT correlation, Opperhuizen 1986)
> 6.0 (estimated, Gobas et al. 1987)
7.06 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.07 (recommended, Sangster 1993)
6.07 (Hansch et al. 1995)
6.07 (GC-RT correlation, Kuramochi et al. 2004)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- 2.95–3.08 mean 3.04 (rainbow trout, wet wt., 15°C, steady-state BCF on 21- to 96-d laboratory study, Oliver & Niimi 1985)
- 1.0 (Kawasaki 1980)
- 5.0 (Nendza 1993)
- 4.892, 4.681 (calculated-MCI, calculated-$K_{OW}$, Lu et al. 1999)

Sorption Partition Coefficient, log $K_{OC}$:
- 4.45, 4.68 (estimated-solubility, Lyman et al. 1982; quoted, $K_{OW}$, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:
- Volatilization: estimated volatilization $t_\frac{1}{2} = 3.3$ d from a model river is 3.3 d, $t_\frac{1}{2} = 114$ months from a model pond with adsorptive processes (Howard 1997)
- Photolysis: not expected to occur (Howard 1997)
- Oxidation: not expected to occur (Howard 1997)
- Hydrolysis: not expected to occur (Howard 1997)

Half-Lives in the Environment:
- Air:
  - Surface water: estimated volatilization $t_\frac{1}{2} = 3.3$ d from a model river, $t_\frac{1}{2} = 114$ months from a model pond with adsorptive processes (Howard 1997)
- Groundwater:
- Sediment:
- Soil:
- Biota:
Common Name: 2-Bromotoluene
Synonym: o-bromotoluene, 1-bromo-2-methylbenzene
Chemical Name: 2-bromotoluene
CAS Registry No: 95-46-5
Molecular Formula: C7H7Br
Molecular Weight: 171.035

Melting Point (°C):
- 27.8 (Weast 1982–82; Lide 2003)

Boiling Point (°C):
181.7 (Dreisbach 1959; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
- 1.4232, 1.41774 (20°C, 25°C, Dreisbach 1959)
- 1.4232 (Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):
120.2 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
49.264, 38.995 (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔHfus (kJ/mol):
2.423 (Dreisbach 1955)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 51.3 (estimated, Howard 1997)
- 1007; 105 (quoted, calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
- 186 (interpolated-Antoine eq., Stuckey & Saylor 1940)
- log P/mmHg = 7.50879 – 1913.46/(T/K – 38.34); temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)
- 133.3* (24.4, summary of lit. data, Stull 1947)
- 181 (calculated by formula., Dreisbach 1955)
- log (P/mmHg) = 6.90847 – 1549.39/(C + t°C); temp range 80–245°C, (Antoine eq. for liquid state, Dreisbach 1955)
- log (P/mmHg) = [–0.2185 x 11365.0/(T/K)] + 8.396578; temp range 24.4–181.8°C (Antoine eq., Weast 1972–73)
- log (P/kPa) = 6.03337 – 1549.39/(T/K – 70.15); temp range 353–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
242 (estimated-group contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log Kow:
- 2.92 (Hansch & Leo 1979, Hansch et al. 1995)
- 3.61 (HPLC-k’ correlation, Hanai et al. 1981)
- 3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log $K_B$:
2.38  (estimated-$K_{ow}$, Howard 1997)

Sorption Partition Coefficient, log $K_{OC}$:
2.96  (estimated, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2} = 1.7$ h from a model river 1-m deep and $t_{1/2} = 14.9$ d from a pond (Howard 1997).
Photolysis:
Oxidation: atmospheric $t_{1/2} \sim 6.2$ d for reaction with hydroxyl radicals in air (Howard 1997).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: atmospheric $t_{1/2} \sim 6.2$ d for reaction with OH radicals in air (Howard 1997).
Surface water: volatilization $t_{1/2} = 1.7$ h from a model river 1-m deep flowing 1 m/s with a wind speed of 5 m/s and $t_{1/2} = 14.9$ d from a model pond with adsorption from water column (Howard 1997).

---

TABLE 6.1.4.10.1
Reported vapor pressures of 2-bromotoluene at various temperatures

| Stull 1947 |
| summary of literature data |
|---|---|
| $t/°C$ | $P/\text{Pa}$ |
| 24.4 | 133.3 |
| 49.7 | 666.6 |
| 62.3 | 1333 |
| 76.0 | 2666 |
| 91.0 | 5333 |
| 100.0 | 7999 |
| 112.0 | 13332 |
| 133.6 | 26664 |
| 157.3 | 53329 |
| 181.8 | 101325 |
| mp/°C | –28 |
6.1.4.11 3-Bromotoluene

Common Name: 3-Bromotoluene
Synonym: m-bromotoluene
Chemical Name: 3-bromotoluene
CAS Registry No: 591-17-3
Molecular Formula: C₇H₇Br
Molecular Weight: 171.035
Melting Point (°C): 
-39.8 (Lide 2003)
Boiling Point (°C): 
183.7 (Lide 2003)
Density (g/cm³ at 20°C): 
1.4099 (Lide 2003)
Molar Volume (cm³/mol): 
121.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_V$ (kJ/mol):
Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
51.3 (estimated, Howard 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (14.8°C, summary of lit. data, Stull 1947)
$\log (P/\text{mmHg}) = 7.75409 - 2049.14/(T/K - 31.44)$; temp range 4–75°C (Antoine eq. based on expbl. data, Hg manometer, Stuckey & Saylor 1940)
$\log (P/\text{mmHg}) = [-0.2185 \times 10537.1/(T/K)] + 7.886560$; temp range 14.8–183.7°C (Antoine eq., Weast 1972–73)
145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_{T}/\text{kPa}) = 6.86228 - 2085.49/(T/K - 27.333)$; temp range: 287–457 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
445 (estimated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, log $K_{OW}$:
3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_{p}$:
2.38 (estimated-$K_{OW}$, Howard 1997)

Sorption Partition Coefficient, log $K_{OC}$:
2.96 (estimated, Howard 1997)
Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.5$ h and $14.9$ d from a model river 1-m deep and $t_{1/2} = 14.9$ d from a pond (Howard 1997).

Photolysis:

Oxidation: atmospheric $t_{1/2} \sim 3$ d for reaction with hydroxyl radical in air (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 3$ d half-life for reaction with hydroxyl radical in air (Howard 1997).

Surface water: volatilization $t_{1/2} = 1.5$ h from a model river 1 m deep flowing 1 m/s with a wind speed of 5 m/s and $t_{1/2} = 14.9$ d in a model pond with adsorption, from water column (Howard 1997).

---

### TABLE 6.1.4.11.1

<table>
<thead>
<tr>
<th>Reported vapor pressures of 3-bromotoluene at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stull 1947</strong></td>
</tr>
<tr>
<td><strong>summary of literature data</strong></td>
</tr>
<tr>
<td>$t/°C$</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>14.8</td>
</tr>
<tr>
<td>50.8</td>
</tr>
<tr>
<td>64.0</td>
</tr>
<tr>
<td>78.1</td>
</tr>
<tr>
<td>93.9</td>
</tr>
<tr>
<td>104.1</td>
</tr>
<tr>
<td>117.8</td>
</tr>
<tr>
<td>138.0</td>
</tr>
<tr>
<td>160.0</td>
</tr>
<tr>
<td>183.7</td>
</tr>
<tr>
<td>mp/°C</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
6.1.4.12 4-Bromotoluene

Common Name: 4-Bromotoluene
Synonym: \(p\)-bromotoluene, 4-bromo-1-methylbenzene
Chemical Name: \(p\)-bromotoluene
CAS Registry No: 106-38-7
Molecular Formula: \(C_7H_7Br\)
Molecular Weight: 171.042
Melting Point (°C):
28.5 (Lide 2003)
Boiling Point (°C):
184.3 (Lide 2003)
Density (g/cm\(^3\) at 25°C):
1.39953 (Dreisbach 1955)
Molar Volume (cm\(^3\)/mol):
122.5 (Ruelle & Kesselring 1997)
141.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
49.74, 39.98 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
14.82 (Dreisbach 1955)
3.5684 (Ruelle & Kesselring 1997)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
110 (Hine & Mookerjee 1975)
110; 81.9 (quoted; calculated-molar volume and mp, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
133.3* (10.3°C, summary of lit. data, Stull 1947)
153.2 (calculated by formula., Dreisbach 1955)
\[
\log (P/mmHg) = 7.00762 – 1612.35/(206.36 + t/°C); \text{ temp range 85–250°C (Antoine eq. for liquid state, Dreisbach 1955)}
\]
\[
\log (P/mmHg) = 7.00762 – 1612.35/(t/°C + 206.36); \text{ temp range 85–280°C (Antoine eq., Dean 1985, 1992)}
\]
\[
\log (P/kPa) = 6.13252 – 1612.35/(T/K – 66.79); \text{ temp range 358–523 K (Antoine eq., Stephenson & Malanowski 1987)}
\]
\[
\log (P/mmHg) = 12.8209 – 2.6568 \times 10^3/(T/K) – 1.4314 \log (T/K) – 8.9677 \times 10^{-4}(T/K) + 3.9733 \times 10^{-7}(T/K)^2; \text{ temp range 300–699 K (Yaws 1994)}
\]
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
23.82 (calculated-P/C, Howard 1997)
Octanol/Water Partition Coefficient, log \(K_{ow}\):
3.42 (quoted, Howard 1997)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.54 (calculated-$K_{OW}$, Howard 1997)

Sorption Partition Coefficient, $\log K_{OC}$:

3.10–3.27 (estimated, Howard 1997)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:

Volatilization:

Photolysis:

Oxidation: $t_\text{½} \sim 9.4$ d for reaction with OH radical in the atmosphere (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_\text{½} \sim 9.4$ d for reaction with OH radical (Howard 1997).

Surface water: volatilization $t_\text{½} = 4.3$ h from a model river 1 m deep and $t_\text{½} = 14.9$ d from an environmental pond (Howard 1997).

---

TABLE 6.1.4.12.1
Reported vapor pressures of 4-bromotoluene at various temperatures
Stull 1947

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.3</td>
<td>133.3</td>
</tr>
<tr>
<td>47.5</td>
<td>666.6</td>
</tr>
<tr>
<td>61.1</td>
<td>1333</td>
</tr>
<tr>
<td>75.2</td>
<td>2666</td>
</tr>
<tr>
<td>91.8</td>
<td>5333</td>
</tr>
<tr>
<td>102.3</td>
<td>7999</td>
</tr>
<tr>
<td>116.4</td>
<td>13332</td>
</tr>
<tr>
<td>137.4</td>
<td>26664</td>
</tr>
<tr>
<td>160.2</td>
<td>53329</td>
</tr>
<tr>
<td>184.5</td>
<td>101325</td>
</tr>
</tbody>
</table>

mp/°C 28.5
6.1.5 IODOBENZENES

6.1.5.1 Iodobenzene

Common Name: Iodobenzene
Synonym: phenyl iodide
Chemical Name: iodobenzene
CAS Registry No: 591-50-4
Molecular Formula: C₆H₅I
Molecular Weight: 204.008
Melting Point (°C):
-31.3 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
188.4 (Lide 2003)
Density (g/cm³ at 20°C):
1.8308 (Weast 1982–83; Lide 2003)
1.8308, 1.8229 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
111.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Wang et al. 1992)
129.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
40.794 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
340 (30°C, Gross et al. 1933)
180 (shake flask-UV spectrophotometry, Andrews & Keefer 1950)
228* (25.1°C, shake flask-spectrophotometry, measured range 10–35°C, Vesala 1973)
229 (shake flask-UV spectrophotometry, Vesala 1974)
158 (Deno & Berkheimer 1960)
95* (shake flask-GC, measured range 5–45.5°C, Nelson & Smit 1978)
267.6* (summary of literature data, temp range 25–50 °C, Horvath 1982)
201 (Miller et al. 1985)
226* (recommended, temp range 10–45°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
S/(g/kg) = 0.59293 – 4.8616 × 10⁻³·(T/K) + 1.21754 × 10⁻⁵·(T/K)²; temp range 283–318 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
213* (29.3°C, Ramsay-Young method, measured range 29.3–100.35°C, Young 1889)
133.3*, 666.6 (24.1, 50.6°C, summary of lit. data, temp range 24.1–188.6°C, Stull 1947)
134.5 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.89506 – 1562.87/(201.0 + t°C); temp range: 85–270°C (Antoine eq. for liquid state, Dreisbach 1955)
132.0 (Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.01187 – 1640.124/(208.765 + t°C); temp range 29.3–188.2°C (Antoine eq. from reported explt. data of Young 1889, Boublik et al. 1973)
134 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.15935 – 1656.226/(210.496 + t/°C); temp range 29.3–188.2°C (Antoine eq. from reported expvl.
data of Young 1889, Bouliblik et al. 1984)
log (P/mmHg) = 7.0119 – 1640.1/(208.8 + t/°C); temp range 20–188°C (Antoine eq., Dean 1985, 1992)
134.5 (Riddick et al. 1986)
133 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.01996 – 1562.87/(– 72.15 + T/K); temp range 358–543 K (Antoine eq.-I, Stephenson & Mal-
anowski 1987)
log (P/kPa) = 6.46493 – 1867.69/(–20.202 + T/K); temp range 462–679 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.36129 – 1765.99/(– 54.15 + T/K); temp range 273–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 32.7342 – 3.5824 × 10³/(T/K) – 8.4197·log (T/K) + 2.0073 × 10–10· ( T / K )+1 .5 9 1×10–6·(T/K)²;
temp range 242–721 K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
130 (recommended, Mackay & Shiu 1981)
134 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log KOW:
3.25, 3.32 (quoted, calculated-fragment const., Rekker 1977)
3.25 (Hansch & Leo 1979)
3.28 (generator column-HPLC, Wasik et al. 1983)
3.28 (generator column-HPLC, Tewari et al. 1982)
3.23 (HPLC/MS correlation, Burkhard et al. 1985)
3.37 (HPLC-RT correlation, Eadsforth 1986)
3.25 (recommended, Sangster 1989)
3.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KOA:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
kOH(calc) = 1.3 × 10–12 cm³ molecule–1 s–1, kOH(obs) = 0.93 × 10–12 cm³ molecule–1 s–1 at room temp. (SAR
structure-activity relationship, Atkinson 1987)
kOH* = (1.32 ± 0.19) × 10–12 cm³ molecule–1 s–1 at 296 K, measured range 234–438 K (flash photolysis-
resonance fluorescence, Wallington et al. 1987)
kOH = 1.32 × 10–12 cm³ molecule–1 s–1; k(soln) = 8.3 × 10–12 cm³ molecule–1 s–1 for reaction with OH radical
in aqueous solution (Wallington et al. 1988)
kOH = 1.10 × 10–12 cm³ molecule–1 s–1, independent of temperature over the range 263–393 K (Atkinson 1989)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
### TABLE 6.1.5.1.1
Reported aqueous solubilities of iodobenzene at various temperatures

\[
S(\text{wt}%) = -2.78956 \times 10^{-3} + 1.95862 \times 10^{-3} \cdot \frac{t}{\degree C} - 4.53984 \times 10^{-5} \cdot \left(\frac{t}{\degree C}\right)^2 + 5.73315 \times 10^{-7} \cdot \left(\frac{t}{\degree C}\right)^3 \tag{1}
\]

\[
S(\text{g/kg}) = 0.59293 - 4.816 \times 10^{-3} \cdot \frac{T}{\text{K}} + 1.21754 \times 10^{-5} \cdot \left(\frac{T}{\text{K}}\right)^2 \tag{2}
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>10</td>
<td>195.29</td>
<td>5</td>
<td>54.9</td>
</tr>
<tr>
<td>15.2</td>
<td>196.56</td>
<td>25</td>
<td>95.0</td>
</tr>
<tr>
<td>19.6</td>
<td>216.42</td>
<td>39</td>
<td>143.8</td>
</tr>
<tr>
<td>25.0</td>
<td>228.45</td>
<td>45.5</td>
<td>207.2</td>
</tr>
<tr>
<td>30.0</td>
<td>236.20</td>
<td>eq. 1</td>
<td>S/wt%</td>
</tr>
<tr>
<td>35.0</td>
<td>251.09</td>
<td>eq. 1</td>
<td>S/wt%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 2</td>
<td>S/(g/kg)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>eq. 2</td>
<td>S/(g/kg)</td>
</tr>
</tbody>
</table>

### FIGURE 6.1.5.1.1
Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for iodobenzene.

© 2006 by Taylor & Francis Group, LLC
TABLE 6.1.5.1.2
Reported vapor pressures of iodobenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \quad \ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \quad \ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>29.3</td>
<td>213</td>
<td>24.1</td>
<td>133.3</td>
</tr>
<tr>
<td>33</td>
<td>240</td>
<td>50.6</td>
<td>666.6</td>
</tr>
<tr>
<td>40.1</td>
<td>367</td>
<td>64</td>
<td>1333</td>
</tr>
<tr>
<td>46.3</td>
<td>513</td>
<td>78.3</td>
<td>2666</td>
</tr>
<tr>
<td>52.5</td>
<td>753</td>
<td>94.4</td>
<td>5333</td>
</tr>
<tr>
<td>57</td>
<td>933</td>
<td>105</td>
<td>7999</td>
</tr>
<tr>
<td>61.45</td>
<td>1187</td>
<td>118.3</td>
<td>13332</td>
</tr>
<tr>
<td>67.8</td>
<td>1627</td>
<td>139.8</td>
<td>26664</td>
</tr>
<tr>
<td>70.9</td>
<td>1927</td>
<td>163.9</td>
<td>53329</td>
</tr>
<tr>
<td>78.4</td>
<td>2700</td>
<td>188.6</td>
<td>101325</td>
</tr>
<tr>
<td>81.9</td>
<td>3166</td>
<td></td>
<td></td>
</tr>
<tr>
<td>85.5</td>
<td>3673</td>
<td></td>
<td></td>
</tr>
<tr>
<td>87.45</td>
<td>4026</td>
<td></td>
<td></td>
</tr>
<tr>
<td>88.75</td>
<td>4266</td>
<td></td>
<td></td>
</tr>
<tr>
<td>91.55</td>
<td>4820</td>
<td></td>
<td></td>
</tr>
<tr>
<td>91.6</td>
<td>4820</td>
<td></td>
<td></td>
</tr>
<tr>
<td>94.75</td>
<td>5466</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100.35</td>
<td>6919</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

complete set of data see ref.

FIGURE 6.1.5.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodobenzene.
6.1.5.2 1,2-Diiodobenzene

Common Name: 1,2-Diiodobenzene
Synonym: o-diiodobenzene
Chemical Name: 1,2-Diiodobenzene
CAS Registry No: 615-42-9
Molecular Formula: C₆H₄I₂
Molecular Weight: 329.051
Melting Point (°C):
Boiling Point (°C):
  287 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  162.6 (calculated-Le Bas method at normal boiling point)
  134.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.956 (mp at 27°C)

Water Solubility (g/m³ or mg/L at 25°C):
  14.9 (shake flask-UV, Andrews & Keefer 1950)
  19.0 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log KOW:
  4.65 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
  4.64 (calculated-fragment const., Yalkowsky et al. 1983)
  4.65; 4.35 (quoted; calculated-molar volume correlation, Wang et al. 1992)
  4.39 (calculated, Müller & Klein 1992)
  4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log KOA:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Half-Lives in the Environment:
6.1.5.3 1,3-Diiodobenzene

Common Name: 1,3-Diiodobenzene
Synonym: m-diiodobenzene
Chemical Name: 1,3-Diiodobenzene
CAS Registry No: 626-00-6
Molecular Formula: C₆H₄I₂
Molecular Weight: 329.905

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
162.6 (calculated-Le Bas method at normal boiling point)
134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔHV (kJ/mol):

Enthalpy of Fusion, ΔHfus (kJ/mol):
3.8064 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.706 (mp at 40.4°C)

Water Solubility (g/m³ or mg/L at 25°C):
9.67 (shake flask-UV, Andrews & Keefer 1950)
8.88 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kow:
4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)
4.39 (calculated, Müller & Klein 1992)
4.70 (calculated-molar volume correlation, Wang et al. 1992)
5.25; 4.56 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log Koa:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Koc:

Environmental Fate Rate Constants, k, or Half-Lives, t½:

Half-Lives in the Environment:
6.1.5.4 1,4-Diiodobenzene

Common Name: 1,4-Diiodobenzene
Synonym: p-diiodobenzene
Chemical Name: 1,4-Diiodobenzene
CAS Registry No: 624-38-4
Molecular Formula: C₆H₄I₂
Molecular Weight: 329.905
Melting Point (°C):
131.5 (Horvath 1982; Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
162.6 (calculated-Le Bas method at normal boiling point)
134.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Entropy of Fusion, ΔSₓᵤₜ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSₕᵤ = 56 J/mol K), F: 0.0902 (mp at 131.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
4.62 (shake flask-UV, Andrews & Keefer 1950)
1.855 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.545 (extrapolated Antoine eq., Stephenson & Malanowski 1987)
log (Pᵥ/kPa) = 8.29504 – 33311.326/(T/K); temp range 372–401 K (Antoine eq-I., solid, Stephenson & Malanowski 1987)
log (Pᵥ/kPa) = 6.8859 – 2747.88/(T/K); temp range 402–560 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒₐₚ:\n4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983; quoted, Wang et al. 1992)
4.39 (calculated, Müller & Klein 1992)
4.11 (shake flask, recommended, Hansch et al. 1995)
4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Kₒₐₐ:\nBioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₒₑ:\nEnvironmental Fate Rate Constants, k, or Half-Lives, tᵯ:\nHalf-Lives in the Environment:
6.1.5.5 1,2,3-Triiodobenzene

Common Name: 1,2,3-Triiodobenzene
Synonym:
Chemical Name: 1,2,3-Triiodobenzene
CAS Registry No: 608-29-7
Molecular Formula: C₆H₃I₃
Molecular Weight: 455.801

Melting Point (°C):
166 (Weast 1982–83, Horvath 1982)

Boiling Point (°C):
sublimation (Weast 1982–83, Horvath 1982)

Density (g/cm³ at 20°C):
141 (Wang et al. 1992)
195.9 (calculated-Le Bas method at normal boiling point)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$), F: 0.041 (mp at 166°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.301 (shake flask-UV, Yalkowsky & Valvani 1980)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
5.86 (quoted, Wang et al. 1992)
6.17; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{\text{OC}}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{\frac{1}{2}}$:

Half-Lives in the Environment:
6.1.5.6 1,2,4-Triiodobenzene

Common Name: 1,2,4-Triiodobenzene  
Synonym:  
Chemical Name: 1,2,4-Triiodobenzene  
CAS Registry No: 615-68-9  
Molecular Formula: C₆H₃I₃  
Molecular Weight: 455.801  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm³ at 20°C):  
Molar Volume (cm³/mol):  
195.9 (calculated-Le Bas method at normal boiling point)  
145 (Wang et al. 1992)  
Dissociation Constant pKₐ:  
Enthalpy of Fusion, ΔH₉₅ (kJ/mol):  
Entropy of Fusion, ΔS₉₅ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS₉₅ = 56 J/mol K), F: 0.223 (mp at 91.5°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
0.538 (shake flask-UV, Yalowsky & Valvani 1980)  
Vapor Pressure (Pa at 25°C):  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log Kₐw:  
5.85 (quoted, Wang et al. 1992)  
6.58; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)  
Octanol/Air Partition Coefficient, log Kₐα:  
Bioconcentration Factor, log BCF:  
Sorption Partition Coefficient, log Kₐc:  
Environmental Fate Rate Constants, k, or Half-Lives, tₕ:  
Half-Lives in the Environment:
6.1.5.7 1,3,5-Triiodobenzene

Common Name: 1,3,5-Triiodobenzene
Synonym: 1,3,5-Triiodobenzene
CAS Registry No: 626-44-8
Molecular Formula: C₆H₃I₃
Molecular Weight: 455.801
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  131  (Wang et al. 1992)
  195.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHᵥₑₑ (kJ/mol):
Entropy of Fusion, ΔSᵥₑₑ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSᵥₑₑ = 56 J/mol K), F: 0.0274 (mp at 184.2°C)
Water Solubility (g/m³ or mg/L at 25°C):
  0.0706  (shake flask-UV, Yalowsky & Valvani 1980)
  0.0644  (quoted, Wang et al. 1992)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐₗₜₚ:
  5.85  (quoted, Wang et al. 1992)
  6.90; 5.82  (predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Kₐₕₐ:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₐₜₜ:
Environmental Fate Rate Constants, k, or Half-Lives, tₑₑ:
Half-Lives in the Environment:
6.1.6 Mixed Halogenated Benzenes

6.1.6.1 2-Bromochlorobenzene

Common Name: 2-Bromochlorobenzene
Synonym: 2-bromo-1-chlorobenzene
Chemical Name:
CAS Registry No: 108-37-2
Molecular Formula: C₆H₄BrCl
Molecular Weight: 191.453
Melting Point (°C):
-12.3 (Weast 1982–83; Horvath 1982; Lide 2003)
Boiling Point (°C):
204 (Weast 1982–83; Horvath 1982; Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
117 (calculated-density, Lande & Banerjee 1981; Wang et al. 1992)
116.8 (Ruelle & Kesselring 1997)
140.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
124 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)
124 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
3.83 (calculated-fragment const., Yalkowsky et al. 1979)
3.86 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983)
3.44 (calculated, Müller & Klein 1992)
3.83; 3.63 (quoted; calculated-molar volume correlation, Wang et al. 1992)
3.83, 3.54; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kbi:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
### 6.1.6.2 3-Bromochlorobenzene

![Chemical Structure](image)

**Common Name:** 3-Bromochlorobenzene  
**Synonym:** m-bromochlorobenzene, 3-bromo-1-chlorobenzene, 1-bromo-3-chlorobenzene  
**Chemical Name:** 3-bromochlorobenzene  
**CAS Registry No.:** 108-37-2  
**Molecular Formula:** C₆H₄BrCl  
**Molecular Weight:** 191.453

**Melting Point (°C):**  
21 (Stephenson & Malanowski 1987)

**Boiling Point (°C):** 196 (Weast 1982-83; Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

**Density (g/cm³):**  
- 1.62745, 1.62065 (20°C, 25°C, Dreisbach & Martin 1949)  
- 1.602 (20°C, Weast 1982-83; Horvath 1982)  
- 1.5771 (20°C, Lide 2003)

**Molar Volume (cm³/mol):**  
- 117.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)  
- 140.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
Enthalpy of Fusion, \( \Delta H_{ fus } \) (kJ/mol):  
Entropy of Fusion, \( \Delta S_{ fus } \) (J/mol K):

**Fugacity Ratio at 25°C, F:** 1.0

**Water Solubility (g/m³ or mg/L at 25°C):**  
- 118 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)  
- 118 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
\[ \log (P/\text{mmHg}) = 7.37230 - 1912.7/(230 + t/°C) \] (Antoine eq., Dreisbach & Martin 1949)  
99.2 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
\[ \log (P_l/\text{kPa}) = 6.4972 - 1912.7/(T/K - 43.15) \] (Antoine eq., liquid, Stephenson & Malanowski 1987)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**

**Octanol/Water Partition Coefficient, log \( K_{ ow } \):**  
- 3.83 (calculated-fragment const., Yalkowsky et al. 1979)  
- 3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)  
- 3.74 (HPLC-k’ correlation, Hanai et al. 1981)  
- 3.72 (calculated, Müller & Klein 1992)  
- 3.61 (calculated-molar volume correlation, Wang et al. 1992)  
- 3.54; 3.36 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

**Octanol/Air Partition Coefficient, log \( K_{ OA } \):**
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:
6.1.6.3 4-Bromochlorobenzene

![Structure of 4-Bromochlorobenzene](image)

**Common Name:** 4-Bromochlorobenzene  
**Synonym:** 4-bromo-1-chlorobenzene, 1-bromo-4-chlorobenzene  
**Chemical Name:** 4-bromochlorobenzene  
**CAS Registry No:** 106-39-8  
**Molecular Formula:** C₆H₄BrCl  
**Molecular Weight:** 191.453

**Melting Point (°C):**  
68  (Weast 1982–83; Horvath 1982; Lide 2003)

**Boiling Point (°C):**  

**Density (g/cm³):**  

**Molar Volume (cm³/mol):**  
121.5  (calculated-density, Stephenson & Malanowski 1987)  
140.2  (calculated-Le Bas method at normal boiling point)  
126.4  (Ruelle & Kesselring 1997)

**Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):**

**Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):**

**Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:** 0.376 (mp at 68°C)

**Water Solubility (g/m³ or mg/L at 25°C):**

44.9; 37.3  (shake flask-UV; calculated-$K_{\text{ow}}$, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983; quoted, Lande & Banerjee 1981; Horvath 1982; Müller & Klein 1992)  
44.9; 37.3  (quoted; calculated-$K_{\text{ow}}$, Valvani & Yalkowsky 1980)  
44.2  (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)  
45; 11.31  (quoted; calculated-molar volume correlation, Wang et al. 1992)  
44.9; 50.4  (quoted; calculated-group contribution method; Kühne et al. 1995)  
44.9; 51.5  (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):**

133.3*  (32.0°C, summary of literature data, temp range 32.0–196.9°C, Stull 1947)  
33.3*  (24.2°C, manometry, measured range 21.4–64.4°C, Walsh & Smith 1961)  
34.45  (interpolated-Antoine eq., Weast 1972–73)  
log (P/mmHg) = [– 0.2185 × 16671.8/(T/K)] + 11.629; temp range 23–63°C (Antoine eq., Weast 1972–73)  
log (P/mmHg) = [– 0.2185 × 11451.1/(T/K)] + 8.222763; temp range 32–196°C (Antoine eq., Weast 1972–73)  
32.12  (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
37.72  (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P/kPa) = 10.478 – 3548.4/(T/K ); temp range 294–337 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)  
log (P/kPa) = 6.71377 – 2074.22/(T/K – 35.248); temp range 333–470 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 3.86 (calculated-fragment const., Yalkowsky et al. 1979)
- 3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983; quoted, Malihot & Peters 1988)
- 3.72 (calculated, Müller & Klein 1992)
- 3.83; 4.29 (quoted; calculated-molar volume correlation, Wang et al. 1992)
- 3.83, 3.73; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

**TABLE 6.1.6.3.1**

Reported vapor pressures of 4-bromochlorobenzene at various temperatures

<table>
<thead>
<tr>
<th>Summary of literature data</th>
<th>Stull 1947</th>
<th>Walsh &amp; Smith 1961</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>32.0</td>
<td>133.3</td>
<td>21.4</td>
</tr>
<tr>
<td>59.5</td>
<td>666.6</td>
<td>24.2</td>
</tr>
<tr>
<td>72.7</td>
<td>1333</td>
<td>26.1</td>
</tr>
<tr>
<td>87.8</td>
<td>2666</td>
<td>29.0</td>
</tr>
<tr>
<td>103.8</td>
<td>5333</td>
<td>30.7</td>
</tr>
<tr>
<td>114.8</td>
<td>7999</td>
<td>35.4</td>
</tr>
<tr>
<td>128.0</td>
<td>13332</td>
<td>35.6</td>
</tr>
<tr>
<td>149.5</td>
<td>26664</td>
<td>40.5</td>
</tr>
<tr>
<td>172.6</td>
<td>53329</td>
<td>40.6</td>
</tr>
<tr>
<td>196.9</td>
<td>10132</td>
<td>44.5</td>
</tr>
<tr>
<td>45.6</td>
<td>221.3</td>
<td>48.9</td>
</tr>
<tr>
<td>49.9</td>
<td>313.3</td>
<td>53.0</td>
</tr>
<tr>
<td>54.7</td>
<td>457.3</td>
<td>57.1</td>
</tr>
<tr>
<td>59.9</td>
<td>673.3</td>
<td>60.7</td>
</tr>
<tr>
<td>64.0</td>
<td>902.6</td>
<td>64.4</td>
</tr>
</tbody>
</table>
FIGURE 6.1.6.3.1 Logarithm of vapor pressure versus reciprocal temperature for 4-bromochlorobenzene.
6.1.6.4  4-Bromoiodobenzene

Common Name: 4-Bromoiodobenzene  
Synonym: 4-bromo-1-iodobenzene  
Chemical Name:  
CAS Registry No: 589-87-7  
Molecular Formula: C₆H₄BrI  
Molecular Weight: 282.904  
Melting Point (°C):  
92  (Weast 1982–83; Horvath 1982; Lide 2003)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
152.6  (calculated-Le Bas method at normal boiling point)  
128.1  (Rulle & Kesselring 1997)  
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):  
19.13  (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ∆Hₜₙₚ (kJ/mol):  
Entropy of Fusion, ∆Sₜₙₚ (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆Sₜₙₚ = 56 J/mol K), F: 0.22 (mp at 92°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
7.8  (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980, Valvani & Yalkowsky 1980)  
7.94  (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)  
Vapor Pressure (Pa at 25°C):  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log Kₐw:  
4.36  (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)  
4.62; 4.10  (predicted; calculated-atom typing scheme, Onel & Iseri 1997)  
4.13  (calculated, Müller & Klein 1992)  
Octanol/Air Partition Coefficient, log Kₐα:  
Bioconcentration Factor, log BCF or log Kₐ:  
Sorption Partition Coefficient, log Kₐ₀C:  
Environmental Fate Rate Constants, k, and Half-Lives, τ₀:  
Half-Lives in the Environment:  

© 2006 by Taylor & Francis Group, LLC
6.1.6.5 2-Chloriodobenzene

![Chemical Structure](image)

Common Name: 2-Chloriodobenzene
Synonym: 2-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 615-41-8
Molecular Formula: ClC₆H₄I
Molecular Weight: 238.453
Melting Point (°C):
0.7  (Weast 1982–83; Horvath 1982; Lide 2003)
Boiling Point (°C):
234.5  (Weast 1982–83; Horvath 1982; Lide 2003)
Density (g/cm³):
1.9515  (Weast 1982–83; Horvath 1982)
1.9255  (20°C, Lide 2003)
Molar Volume (cm³/mol):
150.2  (calculated-Le Bas method at normal boiling point)
134.6  (Rulle & Kesselring 1997)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
68.8  (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
68.68  (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log $K_{ow}$:
4.12  (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)
3.98  (calculated, Müller & Klein 1992)
2.54; 3.89  (quoted; calculated-molar volume correlation, Wang et al. 1992)
4.05, 3.82  (predicted; calculated-atom typing scheme, Onel & Iseri 1997)
Octanol/Air Partition Coefficient, log $K_{oa}$:
Bioconcentration Factor, log BCF or log $K_B$:
Sorption Partition Coefficient, log $K_{oc}$:
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:
6.1.6.6 3-Chloriodobenzene

Common Name: 3-Chloriodobenzene
Synonym: 3-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 625-99-0
Molecular Formula: ClC₆H₄I
Molecular Weight: 238.453
Melting Point (°C):
Boiling Point (°C):
  230  (Weast 1982–83; Lide 2003)
Density (g/cm³):
  1.9515  (25°C, Weast 1982–83)
  1.9255  (20°C, Horvath 1982)
Molar Volume (cm³/mol):
  150.2  (calculated-Le Bas method at normal boiling point)
  124.9  (Rulle & Kesselring 1997)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Fusion, ΔHₐus (kJ/mol):
Entropy of Fusion, ΔSₐus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  68.8  (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
  67.4  (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
  4.12  (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)
  4.05, 3.82  (predicted; calculated-atom typing scheme, Onel & Iseri 1997)
  3.98  (calculated, Müller & Klein 1992)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kb:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
6.1.6.7 4-Chloriodobenzene

Common Name: 4-Chloriodobenzene
Synonym: 4-chloro-1-iodobenzene
Chemical Name:
CAS Registry No: 637-87-6
Molecular Formula: ClC₆H₄I
Molecular Weight: 238.453
Melting Point (°C):
57 (Weast 1982–83; Horvath 1982; Lide 2003)
Boiling Point (°C):
Density (g/cm³):
1.886 (57°C, Weast 1982–83; Horvath 1982)
Molar Volume (cm³/mol):
122 (calculated-density, Lande & Banerjee 1981)
126.4 (Stephenson & Malanowski 19987; Rulle & Kesselring 1997)
127 (Wang et al. 1992)
150.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.4825
Water Solubility (g/m³ or mg/L at 25°C):
22.5 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
31.11 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
16.26 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/P₀) = 8.944–3200/(T/K); temp range 303–323 K (Antoine eq.-I, solid state, Stephenson & Malanowski 1987)
log (P/P₀) = 5.63678 – 1465.651/(T/K – 102.487); temp range 333–500 K (Antoine eq.-II, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C): k’
Octanol/Water Partition Coefficient, log K_{ow}:
4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky)
4.06 (HPLC-k’ correlation, Hanai et al. 1981)
3.98 (calculated, Müller & Klein 1992)
4.47 (calculated-molar volume correlation, Wang et al. 1992)
4.34; 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
### 6.2 SUMMARY TABLES AND QSPR PLOTS

**TABLE 6.2.1**
Summary of physical properties of chlorobenzenes and other halogenated mononuclear aromatics

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Density, ρ g/cm³ at 20°C</th>
<th>Molar volume, V_m cm³/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Chlorobenzenes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>108-90-7</td>
<td>C₆H₅Cl</td>
<td>112.557</td>
<td>−45.31</td>
<td>131.72</td>
<td>1</td>
<td>1.1058</td>
<td>101.79</td>
</tr>
<tr>
<td>1,2-Dichloro-</td>
<td>95-50-1</td>
<td>C₆H₄Cl₂</td>
<td>147.002</td>
<td>−24.8</td>
<td>173</td>
<td>1</td>
<td>1.2884</td>
<td>114.10</td>
</tr>
<tr>
<td>1,3-Dichloro-</td>
<td>541-73-1</td>
<td>C₆H₄Cl₂</td>
<td>147.002</td>
<td>−17.0</td>
<td>180</td>
<td>1</td>
<td>1.3059</td>
<td>112.57</td>
</tr>
<tr>
<td>1,4-Dichloro-</td>
<td>106-46-7</td>
<td>C₆H₄Cl₂</td>
<td>147.002</td>
<td>53.09</td>
<td>174</td>
<td>0.530</td>
<td>1.2457</td>
<td>118.01</td>
</tr>
<tr>
<td>1,2,3-Trichloro-</td>
<td>87-61-6</td>
<td>C₆H₃Cl₃</td>
<td>181.447</td>
<td>−17.0</td>
<td>180</td>
<td>1</td>
<td>1.3059</td>
<td>114.10</td>
</tr>
<tr>
<td>1,2,4-Trichloro-</td>
<td>120-82-1</td>
<td>C₆H₃Cl₃</td>
<td>181.447</td>
<td>−24.8</td>
<td>173</td>
<td>1</td>
<td>1.2884</td>
<td>114.10</td>
</tr>
<tr>
<td>1,3,5-Trichloro-</td>
<td>108-70-3</td>
<td>C₆H₃Cl₃</td>
<td>181.447</td>
<td>−17.0</td>
<td>180</td>
<td>1</td>
<td>1.3059</td>
<td>114.10</td>
</tr>
<tr>
<td>1,2,3,4-Tetrachloro-</td>
<td>634-66-2</td>
<td>C₆H₂Cl₄</td>
<td>215.892</td>
<td>−17.0</td>
<td>180</td>
<td>1</td>
<td>1.3059</td>
<td>114.10</td>
</tr>
<tr>
<td>1,2,3,5-Tetrachloro-</td>
<td>634-90-2</td>
<td>C₆H₂Cl₄</td>
<td>215.892</td>
<td>−24.8</td>
<td>173</td>
<td>1</td>
<td>1.2884</td>
<td>114.10</td>
</tr>
<tr>
<td>1,2,4,5-Tetrachloro-</td>
<td>95-94-3</td>
<td>C₆H₂Cl₄</td>
<td>215.892</td>
<td>−17.0</td>
<td>180</td>
<td>1</td>
<td>1.3059</td>
<td>114.10</td>
</tr>
<tr>
<td>Pentachlorobenzene</td>
<td>608-93-5</td>
<td>C₆Cl₅</td>
<td>250.337</td>
<td>86</td>
<td>277</td>
<td>0.525</td>
<td>1.2457</td>
<td>118.01</td>
</tr>
<tr>
<td>Hexachlorobenzene</td>
<td>118-74-1</td>
<td>C₆Cl₆</td>
<td>284.782</td>
<td>228.83</td>
<td>325</td>
<td>0.0100</td>
<td>1.2457</td>
<td>118.01</td>
</tr>
<tr>
<td><strong>Chlorotoluenes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-Chlorotoluene</td>
<td>95-49-8</td>
<td>C₇H₇Cl</td>
<td>126.584</td>
<td>−35.8</td>
<td>159.0</td>
<td>1</td>
<td>1.0825</td>
<td>116.94</td>
</tr>
<tr>
<td>3-Chlorotoluene</td>
<td>108-41-8</td>
<td>C₇H₇Cl</td>
<td>126.584</td>
<td>−47.8</td>
<td>161.8</td>
<td>1</td>
<td>1.0722</td>
<td>118.06</td>
</tr>
<tr>
<td>4-Chlorotoluene</td>
<td>106-43-4</td>
<td>C₇H₇Cl</td>
<td>126.584</td>
<td>−13.5</td>
<td>201</td>
<td>1</td>
<td>1.2476</td>
<td>129.07</td>
</tr>
<tr>
<td>2,4-Dichlorotoluene</td>
<td>95-73-8</td>
<td>C₇H₆Cl₂</td>
<td>161.029</td>
<td>−17.0</td>
<td>201</td>
<td>1</td>
<td>1.2476</td>
<td>129.07</td>
</tr>
<tr>
<td>2,6-Dichlorotoluene</td>
<td>118-69-4</td>
<td>C₇H₆Cl₂</td>
<td>161.029</td>
<td>−13.5</td>
<td>201</td>
<td>1</td>
<td>1.2476</td>
<td>129.07</td>
</tr>
<tr>
<td>3,4-Dichlorotoluene</td>
<td>95-75-0</td>
<td>C₇H₆Cl₂</td>
<td>161.029</td>
<td>−15.2</td>
<td>208.9</td>
<td>1</td>
<td>1.2564</td>
<td>128.17</td>
</tr>
<tr>
<td>2,3,6-Trichlorotoluene</td>
<td>2077-46-5</td>
<td>C₇H₅Cl₃</td>
<td>195.474</td>
<td>45.5</td>
<td>229.5</td>
<td>0.629</td>
<td>1.2476</td>
<td>129.07</td>
</tr>
<tr>
<td>2,4,5-Trichlorotoluene</td>
<td>6639-30-1</td>
<td>C₇H₅Cl₃</td>
<td>195.474</td>
<td>82.4</td>
<td>231</td>
<td>0.273</td>
<td>1.2476</td>
<td>129.07</td>
</tr>
<tr>
<td>α-Chlorotoluene</td>
<td>100-44-7</td>
<td>C₇H₅Cl</td>
<td>126.584</td>
<td>−45</td>
<td>179</td>
<td>1</td>
<td>1.1004</td>
<td>115.03</td>
</tr>
<tr>
<td>α, α, α-Trichlorotoluene</td>
<td>98-07-7</td>
<td>C₇H₅Cl₃</td>
<td>195.474</td>
<td>−4.42</td>
<td>221</td>
<td>1</td>
<td>1.3723</td>
<td>142.44</td>
</tr>
<tr>
<td>Pentachlorotoluene</td>
<td>877-11-2</td>
<td>C₇H₅Cl₃</td>
<td>264.364</td>
<td>224.8</td>
<td>301</td>
<td>0.0110</td>
<td>1.3723</td>
<td>142.44</td>
</tr>
<tr>
<td>o-Chlorostyrene</td>
<td>2039-87-4</td>
<td>C₈H₇Cl</td>
<td>138.595</td>
<td>−63.1</td>
<td>188.7</td>
<td>1</td>
<td>1.1000</td>
<td>126.00</td>
</tr>
<tr>
<td>m-Chlorostyrene</td>
<td>2039-85-2</td>
<td>C₈H₇Cl</td>
<td>138.595</td>
<td>−63.1</td>
<td>188.7</td>
<td>1</td>
<td>1.1000</td>
<td>126.00</td>
</tr>
<tr>
<td>p-Chlorostyrene</td>
<td>1073-67-2</td>
<td>C₈H₇Cl</td>
<td>138.595</td>
<td>15.9</td>
<td>192</td>
<td>1</td>
<td>1.0868</td>
<td>127.53</td>
</tr>
<tr>
<td>Octachlorostyrene</td>
<td>29082-74-4</td>
<td>C₈Cl₄</td>
<td>379.710</td>
<td>99</td>
<td>0.188</td>
<td>0.188</td>
<td>1.0868</td>
<td>127.53</td>
</tr>
</tbody>
</table>

(Continued)
TABLE 6.2.1 (Continued)

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Density, ρ g/cm³ at 20°C</th>
<th>Molar volume, V_m cm³/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluorobenzenes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fluorobenzene</td>
<td>462-06-6</td>
<td>C₆H₅F</td>
<td>96.102</td>
<td>-42.18</td>
<td>84.73</td>
<td>1</td>
<td>1.0225</td>
<td>93.99</td>
</tr>
<tr>
<td>1,2-Difluorobenzene</td>
<td>367-11-3</td>
<td>C₆H₄F₂</td>
<td>114.093</td>
<td>-47.1</td>
<td>94</td>
<td>1</td>
<td>1.158</td>
<td>98.53</td>
</tr>
<tr>
<td>1,3-Difluorobenzene</td>
<td>372-18-9</td>
<td>C₆H₄F₂</td>
<td>114.093</td>
<td>-69.12</td>
<td>82.6</td>
<td>1</td>
<td>1.1572</td>
<td>98.59</td>
</tr>
<tr>
<td>1,4-Difluorobenzene</td>
<td>540-36-3</td>
<td>C₆H₄F₂</td>
<td>114.093</td>
<td>-23.55</td>
<td>89</td>
<td>1</td>
<td>1.1701</td>
<td>97.51</td>
</tr>
<tr>
<td>1,2,4-Trifluorobenzene</td>
<td>367-23-7</td>
<td>C₆H₃F₃</td>
<td>132.083</td>
<td>-5.5</td>
<td>75.5</td>
<td>1</td>
<td>103.4†</td>
<td>111.0</td>
</tr>
<tr>
<td>1,3,5-Trifluorobenzene</td>
<td>372-38-3</td>
<td>C₆H₃F₃</td>
<td>132.083</td>
<td>90</td>
<td></td>
<td>1</td>
<td>107.7†</td>
<td>116.0</td>
</tr>
<tr>
<td>1,2,3,4-Tetrafluorobenzene</td>
<td>2367-82-0</td>
<td>C₆H₂F₄</td>
<td>150.074</td>
<td>-46.25</td>
<td>84.4</td>
<td>1</td>
<td>1.158</td>
<td>126.45</td>
</tr>
<tr>
<td>1,2,3,5-Tetrafluorobenzene</td>
<td>771-56-2</td>
<td>C₆H₂F₄</td>
<td>150.074</td>
<td>3.88</td>
<td>90.2</td>
<td>1</td>
<td>1.4255</td>
<td>126.45</td>
</tr>
<tr>
<td>1,2,4,5-Tetrafluorobenzene</td>
<td>327-54-8</td>
<td>C₆H₂F₄</td>
<td>150.074</td>
<td>7.0</td>
<td>218.5</td>
<td>0.244</td>
<td>2.6580</td>
<td>116.0</td>
</tr>
<tr>
<td>Pentafluorobenzene</td>
<td>363-72-4</td>
<td>C₆F₅</td>
<td>168.064</td>
<td>-47.4</td>
<td>85.74</td>
<td>1</td>
<td>1.4255</td>
<td>126.45</td>
</tr>
<tr>
<td>Hexafluorobenzene</td>
<td>392-56-3</td>
<td>C₆F₆</td>
<td>180.054</td>
<td>5.03</td>
<td>80.26</td>
<td>1</td>
<td>1.6184</td>
<td>116.0</td>
</tr>
<tr>
<td>Pentafluorotoluene</td>
<td>771-56-2</td>
<td>C₇H₃F₅</td>
<td>182.091</td>
<td>-29.78</td>
<td>117.5</td>
<td>1</td>
<td>1.440</td>
<td>126.45</td>
</tr>
<tr>
<td>Chloropentafluorobenzene</td>
<td>344-07-0</td>
<td>C₆ClF₅</td>
<td>202.509</td>
<td>37.5</td>
<td>145.6</td>
<td>0.754</td>
<td>141.9</td>
<td></td>
</tr>
<tr>
<td>Pentafluorophenol</td>
<td>771-61-9</td>
<td>C₆F₅O</td>
<td>184.063</td>
<td>35.7</td>
<td>145.6</td>
<td>0.754</td>
<td>128.4</td>
<td></td>
</tr>
<tr>
<td><strong>Bromobenzenes and bromotoluenes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bromobenzene</td>
<td>108-86-1</td>
<td>C₆H₅Br</td>
<td>157.008</td>
<td>-30.72</td>
<td>156.06</td>
<td>1</td>
<td>1.4950</td>
<td>119.3</td>
</tr>
<tr>
<td>1,2-Dibromobenzene</td>
<td>583-53-9</td>
<td>C₆H₅Br₂</td>
<td>235.904</td>
<td>7</td>
<td>225</td>
<td>1</td>
<td>1.9843</td>
<td>142.6</td>
</tr>
<tr>
<td>1,3-Dibromobenzene</td>
<td>108-36-1</td>
<td>C₆H₅Br₂</td>
<td>235.904</td>
<td>-7.0</td>
<td>218.5</td>
<td>1</td>
<td>1.9523</td>
<td>120.83</td>
</tr>
<tr>
<td>1,4-Dibromobenzene</td>
<td>106-37-6</td>
<td>C₆H₅Br₂</td>
<td>235.904</td>
<td>87.43</td>
<td>218.5</td>
<td>0.244</td>
<td>1.5742</td>
<td>149.86</td>
</tr>
<tr>
<td>1,2,3-Tribromobenzene</td>
<td>608-21-9</td>
<td>C₆H₅Br₃</td>
<td>314.800</td>
<td>87.8</td>
<td>275</td>
<td>0.644</td>
<td>165.9</td>
<td></td>
</tr>
<tr>
<td>1,2,4-Tribromobenzene</td>
<td>615-54-3</td>
<td>C₆H₅Br₃</td>
<td>314.800</td>
<td>44.5</td>
<td>275</td>
<td>0.644</td>
<td>165.9</td>
<td></td>
</tr>
<tr>
<td>1,3,5-Tribromobenzene</td>
<td>626-39-1</td>
<td>C₆H₅Br₃</td>
<td>314.800</td>
<td>122.8</td>
<td>271</td>
<td>0.110</td>
<td>165.9</td>
<td></td>
</tr>
<tr>
<td>1,2,4,5-Tetra bromobenzene</td>
<td>636-28-2</td>
<td>C₆H₅Br₄</td>
<td>393.696</td>
<td>182</td>
<td>0.0288</td>
<td>3.0720</td>
<td>128.16</td>
<td>189.2</td>
</tr>
<tr>
<td>Hexabromobenzene</td>
<td>87-82-1</td>
<td>C₆Br₆</td>
<td>351.88</td>
<td>157.008</td>
<td>327</td>
<td>0.0011</td>
<td>235.8</td>
<td></td>
</tr>
<tr>
<td>2-Bromotoluene</td>
<td>95-46-5</td>
<td>C₇H₇Br</td>
<td>171.035</td>
<td>-27.8</td>
<td>181.7</td>
<td>1</td>
<td>1.4232</td>
<td>120.18</td>
</tr>
<tr>
<td>3-Bromotoluene</td>
<td>591-17-3</td>
<td>C₇H₇Br</td>
<td>171.035</td>
<td>-39.8</td>
<td>183.7</td>
<td>1</td>
<td>1.4099</td>
<td>121.31</td>
</tr>
<tr>
<td>4-Bromotoluene</td>
<td>106-38-7</td>
<td>C₇H₇Br</td>
<td>171.035</td>
<td>28.5</td>
<td>184.3</td>
<td>1</td>
<td>141.5</td>
<td></td>
</tr>
<tr>
<td><strong>Iodobenzenes:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iodobenzene</td>
<td>591-50-4</td>
<td>C₆H₅I</td>
<td>204.008</td>
<td>-31.3</td>
<td>188.4</td>
<td>1</td>
<td>1.8308</td>
<td>129.3</td>
</tr>
<tr>
<td>1,2-Diodobenzene</td>
<td>615-42-9</td>
<td>C₆H₅I₂</td>
<td>329.905</td>
<td>27</td>
<td>287</td>
<td>0.956</td>
<td>2.5400</td>
<td>129.88</td>
</tr>
<tr>
<td>1,3-Diodobenzene</td>
<td>626-00-6</td>
<td>C₆H₅I₂</td>
<td>329.905</td>
<td>40.4</td>
<td>285</td>
<td>0.706</td>
<td>162.6</td>
<td></td>
</tr>
<tr>
<td>1,4-Diodobenzene</td>
<td>624-38-4</td>
<td>C₆H₅I₂</td>
<td>329.905</td>
<td>131.5</td>
<td>285</td>
<td>0.0902</td>
<td>162.6</td>
<td></td>
</tr>
</tbody>
</table>
### Table 6.2.2

Summary of selected physical-chemical properties of chlorobenzenes and other halogenated mononuclear aromatics at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P/Pa</td>
<td>P_/Pa</td>
<td>S/(g/m³)</td>
</tr>
<tr>
<td>Chlorobenzenes:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>1580</td>
<td>1580</td>
<td>484</td>
</tr>
<tr>
<td>1,2-Dichloro-</td>
<td>170</td>
<td>170</td>
<td>140</td>
</tr>
<tr>
<td>1,3-Dichloro-</td>
<td>260</td>
<td>260</td>
<td>120</td>
</tr>
<tr>
<td>1,4-Dichloro-</td>
<td>130</td>
<td>245</td>
<td>80</td>
</tr>
<tr>
<td>1,2,3-Trichloro-</td>
<td>28</td>
<td>50.72</td>
<td>21</td>
</tr>
<tr>
<td>1,2,4-Trichloro-</td>
<td>40</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>1,3,5-Trichloro-</td>
<td>25</td>
<td>78.05</td>
<td>5.3</td>
</tr>
<tr>
<td>1,2,3,4-Tetrachloro-</td>
<td>4.0</td>
<td>6.64</td>
<td>7.8</td>
</tr>
<tr>
<td>1,2,3,5-Tetrachloro-</td>
<td>9.8</td>
<td>19.01</td>
<td>3.6</td>
</tr>
<tr>
<td>1,2,4,5-Tetrachloro-</td>
<td>0.72</td>
<td>9.56</td>
<td>1.27</td>
</tr>
<tr>
<td>Pentachlorobenzene</td>
<td>0.22</td>
<td>0.8730</td>
<td>0.65</td>
</tr>
<tr>
<td>Hexachlorobenzene</td>
<td>0.0023</td>
<td>0.23</td>
<td>0.005</td>
</tr>
</tbody>
</table>

* Assuming ∆S<sub>fus</sub> = 56 J/mol K

(a) ‡ Chiou 1985 (liquid molar volume), † Stephenson & Malanowski 1987, §Wang et al. 1992, and calculated as MW/p at 20°C for this work
### TABLE 6.2.3
Suggested half-life classes of chlorobenzenes and other halogenated mononuclear aromatics in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorobenzene</td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2-Dichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,3-Dichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,4-Dichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,3-Trichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,4-Trichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,3,5-Trichloro-</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,3,4-Tetrachloro-</td>
<td>6</td>
<td>7</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,3,5-Tetrachloro-</td>
<td>6</td>
<td>7</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,4,5-Tetrachloro-</td>
<td>6</td>
<td>7</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Pentachlorobenzene</td>
<td>7</td>
<td>8</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Hexachlorobenzene</td>
<td>8</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Fluorobenzene</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>Bromobenzene</td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Iodobenzene</td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
</tbody>
</table>

where,

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>&lt;10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~1 day)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~2 days)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1,700 (~2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5,500 (~8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17,000 (~2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55,000 (~6 years)</td>
<td>&gt;30,000</td>
</tr>
</tbody>
</table>

**FIGURE 6.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.
FIGURE 6.2.2  Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.

FIGURE 6.2.3  Octanol-water partition coefficient versus Le Bas molar volume for chlorobenzenes.
FIGURE 6.2.4 Henry’s law constant versus Le Bas molar volume for chlorobenzenes.

FIGURE 6.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) chlorobenzenes.
6.3 REFERENCES


Chlorobenzenes and Other Halogenated Mononuclear Aromatics


Sangster, J. (1993) LOGKOW database, Sangster Research Laboratories, Montreal, Quebec, Canada.


Simmons, P., Branson, D., Bailey, R.I. (1976) 1,2,4-Trichlorobenzene-biodegradable or not? \textit{Canadian Assoc. of Textile Colourists} and Chemists. International Technical Conference. Quebec, Canada.


7 Polychlorinated Biphenyls (PCBs)

CONTENTS

7.1 List of Chemicals and Data Compilations .......................... 1484
    7.1.1 PCB congeners ........................................... 1484
        7.1.1.0 Biphenyl ........................................ 1484
        7.1.1.1 2-Chlorobiphenyl (PCB-1) .......................... 1492
        7.1.1.2 3-Chlorobiphenyl (PCB-2) .......................... 1497
        7.1.1.3 4-Chlorobiphenyl (PCB-3) .......................... 1501
        7.1.1.4 2,2’-Dichlorobiphenyl (PCB-4) ...................... 1508
        7.1.1.5 2,3-Dichlorobiphenyl (PCB-5) ....................... 1511
        7.1.1.6 2,3’-Dichlorobiphenyl (PCB-6) ...................... 1514
        7.1.1.7 2,4-Dichlorobiphenyl (PCB-7) ....................... 1516
        7.1.1.8 2,4’-Dichlorobiphenyl (PCB-8) ...................... 1519
        7.1.1.9 2,5-Dichlorobiphenyl (PCB-9) ....................... 1522
        7.1.1.10 2,6-Dichlorobiphenyl (PCB-10) ..................... 1525
        7.1.1.11 3,3’-Dichlorobiphenyl (PCB-11) ................... 1528
        7.1.1.12 3,4-Dichlorobiphenyl (PCB-12) .................... 1530
        7.1.1.13 3,4’-Dichlorobiphenyl (PCB-13) ................... 1533
        7.1.1.14 3,5-Dichlorobiphenyl (PCB-14) .................... 1535
        7.1.1.15 4,4’-Dichlorobiphenyl (PCB-15) ................... 1537
        7.1.1.16 2,2’,3-Trichlorobiphenyl (PCB-16) ............... 1542
        7.1.1.17 2,2’,4-Trichlorobiphenyl (PCB-17) ............... 1545
        7.1.1.18 2,2’,5-Trichlorobiphenyl (PCB-18) ............... 1547
        7.1.1.19 2,2’,6-Trichlorobiphenyl (PCB-19) ............... 1551
        7.1.1.20 2,3,3’-Trichlorobiphenyl (PCB-20) ............... 1553
        7.1.1.21 2,3,4-Trichlorobiphenyl (PCB-21) ............... 1555
        7.1.1.22 2,3,4’-Trichlorobiphenyl (PCB-22) ............... 1557
        7.1.1.23 2,3,5-Trichlorobiphenyl (PCB-23) ............... 1559
        7.1.1.24 2,3,6-Trichlorobiphenyl (PCB-24) ............... 1561
        7.1.1.25 2,3’,4-Trichlorobiphenyl (PCB-25) ............... 1564
        7.1.1.26 2,3’,5-Trichlorobiphenyl (PCB-26) ............... 1566
        7.1.1.27 2,3’,6-Trichlorobiphenyl (PCB-27) ............... 1568
        7.1.1.28 2,4,4’-Trichlorobiphenyl (PCB-28) ............... 1570
        7.1.1.29 2,4,5-Trichlorobiphenyl (PCB-29) ............... 1574
        7.1.1.30 2,4,6-Trichlorobiphenyl (PCB-30) ............... 1578
        7.1.1.31 2,4’,5-Trichlorobiphenyl (PCB-31) ............... 1580
        7.1.1.32 2,4’,6-Trichlorobiphenyl (PCB-32) ............... 1584
        7.1.1.33 2,3’,4’-Trichlorobiphenyl (PCB-33) ............. 1586
        7.1.1.34 2,3’,5-Trichlorobiphenyl (PCB-34) ............... 1589
        7.1.1.35 3,3’,4-Trichlorobiphenyl (PCB-35) ............... 1591
        7.1.1.36 3,3’,5-Trichlorobiphenyl (PCB-36) ............... 1593
        7.1.1.37 3,4,4’-Trichlorobiphenyl (PCB-37) ............... 1595
        7.1.1.38 3,4,5-Trichlorobiphenyl (PCB-38) ............... 1597
| 7.1.1.39 | 3',4',5'-Trichlorobiphenyl (PCB-39) | 1599 |
| 7.1.1.40 | 2',2',3',3'-Tetrachlorobiphenyl (PCB-40) | 1601 |
| 7.1.1.41 | 2',2',3',4'-Tetrachlorobiphenyl (PCB-41) | 1604 |
| 7.1.1.42 | 2',2',3',5'-Tetrachlorobiphenyl (PCB-42) | 1606 |
| 7.1.1.43 | 2',2',3',6'-Tetrachlorobiphenyl (PCB-43) | 1608 |
| 7.1.1.44 | 2',2',3',5'-Tetrachlorobiphenyl (PCB-44) | 1610 |
| 7.1.1.45 | 2',2',3',6'-Tetrachlorobiphenyl (PCB-45) | 1613 |
| 7.1.1.46 | 2',2',4',4'-Tetrachlorobiphenyl (PCB-47) | 1615 |
| 7.1.1.47 | 2',2',4',5'-Tetrachlorobiphenyl (PCB-48) | 1617 |
| 7.1.1.48 | 2',2',4',5'-Tetrachlorobiphenyl (PCB-49) | 1620 |
| 7.1.1.49 | 2',2',4',6'-Tetrachlorobiphenyl (PCB-50) | 1622 |
| 7.1.1.50 | 2',2',4',6'-Tetrachlorobiphenyl (PCB-51) | 1625 |
| 7.1.1.51 | 2',2',4',5'-Tetrachlorobiphenyl (PCB-52) | 1627 |
| 7.1.1.52 | 2',2',4',6'-Tetrachlorobiphenyl (PCB-53) | 1629 |
| 7.1.1.53 | 2',2',4',6'-Tetrachlorobiphenyl (PCB-54) | 1632 |
| 7.1.1.54 | 2',2',4',6'-Tetrachlorobiphenyl (PCB-55) | 1634 |
| 7.1.1.55 | 2',3',4'-Tetrachlorobiphenyl (PCB-56) | 1641 |
| 7.1.1.56 | 2',3',4'-Tetrachlorobiphenyl (PCB-57) | 1643 |
| 7.1.1.57 | 2',3',4'-Tetrachlorobiphenyl (PCB-58) | 1645 |
| 7.1.1.58 | 2',3',4'-Tetrachlorobiphenyl (PCB-59) | 1647 |
| 7.1.1.59 | 2',3',4'-Tetrachlorobiphenyl (PCB-60) | 1649 |
| 7.1.1.60 | 2',3',4'-Tetrachlorobiphenyl (PCB-61) | 1651 |
| 7.1.1.61 | 2',3',4'-Tetrachlorobiphenyl (PCB-62) | 1653 |
| 7.1.1.62 | 2',3',4'-Tetrachlorobiphenyl (PCB-63) | 1655 |
| 7.1.1.63 | 2',3',4'-Tetrachlorobiphenyl (PCB-64) | 1657 |
| 7.1.1.64 | 2',3',4'-Tetrachlorobiphenyl (PCB-65) | 1659 |
| 7.1.1.65 | 2',3',4'-Tetrachlorobiphenyl (PCB-66) | 1661 |
| 7.1.1.66 | 2',3',4'-Tetrachlorobiphenyl (PCB-67) | 1663 |
| 7.1.1.67 | 2',3',4'-Tetrachlorobiphenyl (PCB-68) | 1665 |
| 7.1.1.68 | 2',3',4'-Tetrachlorobiphenyl (PCB-69) | 1667 |
| 7.1.1.69 | 2',3',4'-Tetrachlorobiphenyl (PCB-70) | 1669 |
| 7.1.1.70 | 2',3',4'-Tetrachlorobiphenyl (PCB-71) | 1671 |
| 7.1.1.71 | 2',3',4'-Tetrachlorobiphenyl (PCB-72) | 1673 |
| 7.1.1.72 | 2',3',4'-Tetrachlorobiphenyl (PCB-73) | 1675 |
| 7.1.1.73 | 2',3',4'-Tetrachlorobiphenyl (PCB-74) | 1677 |
| 7.1.1.74 | 2',3',4'-Tetrachlorobiphenyl (PCB-75) | 1679 |
| 7.1.1.75 | 2',3',4'-Tetrachlorobiphenyl (PCB-76) | 1681 |
| 7.1.1.76 | 2',3',4'-Tetrachlorobiphenyl (PCB-77) | 1683 |
| 7.1.1.77 | 2',3',4'-Tetrachlorobiphenyl (PCB-78) | 1685 |
| 7.1.1.78 | 2',3',4'-Tetrachlorobiphenyl (PCB-79) | 1687 |
| 7.1.1.79 | 2',3',4'-Tetrachlorobiphenyl (PCB-80) | 1689 |
| 7.1.1.80 | 2',3',4'-Tetrachlorobiphenyl (PCB-81) | 1691 |
| 7.1.1.81 | 2',3',4'-Tetrachlorobiphenyl (PCB-82) | 1693 |
| 7.1.1.82 | 2',3',4'-Tetrachlorobiphenyl (PCB-83) | 1695 |
| 7.1.1.83 | 2',3',4'-Tetrachlorobiphenyl (PCB-84) | 1697 |
| 7.1.1.84 | 2',3',4'-Tetrachlorobiphenyl (PCB-85) | 1699 |
| 7.1.1.85 | 2',3',4'-Tetrachlorobiphenyl (PCB-86) | 1701 |
| 7.1.1.86 | 2',3',4'-Tetrachlorobiphenyl (PCB-87) | 1703 |
| 7.1.1.87 | 2',3',4'-Tetrachlorobiphenyl (PCB-88) | 1705 |
| 7.1.1.88 | 2',3',4'-Tetrachlorobiphenyl (PCB-89) | 1707 |
| 7.1.1.89 | 2',3',4'-Tetrachlorobiphenyl (PCB-90) | 1709 |
| 7.1.1.90 | 2',3',4'-Tetrachlorobiphenyl (PCB-91) | 1711 |
| 7.1.1.91 | 2',3',4'-Tetrachlorobiphenyl (PCB-92) | 1713 |
| 7.1.1.92 | 2',3',4'-Tetrachlorobiphenyl (PCB-93) | 1715 |
| 7.1.1.93 | 2',3',4'-Tetrachlorobiphenyl (PCB-94) | 1717 |
Polychlorinated Biphenyls (PCBs)

7.1.1.94 2,2',3,5,6'-Pentachlorobiphenyl (PCB-94) .................................................. 1731
7.1.1.95 2,2',3,5'-6-Pentachlorobiphenyl (PCB-95) .................................................. 1733
7.1.1.96 2,2',3,6,6'-Pentachlorobiphenyl (PCB-96) .................................................. 1736
7.1.1.97 2,2',3,4,5'-Pentachlorobiphenyl (PCB-97) .................................................. 1738
7.1.1.98 2,2',3,4,6'-Pentachlorobiphenyl (PCB-98) .................................................. 1741
7.1.1.99 2,2',4,4'-5-Pentachlorobiphenyl (PCB-99) .................................................. 1743
7.1.1.100 2,2',4,4',6-Pentachlorobiphenyl (PCB-100) .............................................. 1746
7.1.1.101 2,2',4,5,5'-Pentachlorobiphenyl (PCB-101) .............................................. 1748
7.1.1.102 2,2',4,5,6'-Pentachlorobiphenyl (PCB-102) .............................................. 1755
7.1.1.103 2,2',4,5',6-Pentachlorobiphenyl (PCB-103) .............................................. 1757
7.1.1.104 2,2',4,6,6'-Pentachlorobiphenyl (PCB-104) .............................................. 1759
7.1.1.105 2,3',3',4,4'-Pentachlorobiphenyl (PCB-105) .............................................. 1761
7.1.1.106 2,3',3',4,5-Pentachlorobiphenyl (PCB-106) .............................................. 1765
7.1.1.107 2,3',3',4,5,5-Pentachlorobiphenyl (PCB-107) .............................................. 1767
7.1.1.108 2,3',3',4,5'-Pentachlorobiphenyl (PCB-108) .............................................. 1769
7.1.1.109 2,3',3',4,6-Pentachlorobiphenyl (PCB-109) .............................................. 1771
7.1.1.110 2,3',3',4,6-Pentachlorobiphenyl (PCB-110) .............................................. 1773
7.1.1.111 2,3',3',5,5'-Pentachlorobiphenyl (PCB-111) .............................................. 1776
7.1.1.112 2,3',3',5,6-Pentachlorobiphenyl (PCB-112) .............................................. 1778
7.1.1.113 2,3',3',5,6-Pentachlorobiphenyl (PCB-113) .............................................. 1780
7.1.1.114 2,3',4,4',5-Pentachlorobiphenyl (PCB-114) .............................................. 1782
7.1.1.115 2,3',4,4',6-Pentachlorobiphenyl (PCB-115) .............................................. 1784
7.1.1.116 2,3',4,5,6-Pentachlorobiphenyl (PCB-116) .............................................. 1786
7.1.1.117 2,3',4,5,6-Pentachlorobiphenyl (PCB-117) .............................................. 1788
7.1.1.118 2,3',4,4',5-Pentachlorobiphenyl (PCB-118) .............................................. 1790
7.1.1.119 2,3',4,4',6-Pentachlorobiphenyl (PCB-119) .............................................. 1794
7.1.1.120 2,3',4,5,5'-Pentachlorobiphenyl (PCB-120) .............................................. 1796
7.1.1.121 2,3',4,5,5'-Pentachlorobiphenyl (PCB-121) .............................................. 1798
7.1.1.122 2,3',4,5,6-Pentachlorobiphenyl (PCB-122) .............................................. 1800
7.1.1.123 2,3',4,4',5-Pentachlorobiphenyl (PCB-123) .............................................. 1802
7.1.1.124 2,3',4,5,5'-Pentachlorobiphenyl (PCB-124) .............................................. 1804
7.1.1.125 2,3',4,5,6-Pentachlorobiphenyl (PCB-125) .............................................. 1806
7.1.1.126 2,3',4,4',5-Pentachlorobiphenyl (PCB-126) .............................................. 1808
7.1.1.127 2,3',4,4',6-Pentachlorobiphenyl (PCB-127) .............................................. 1811
7.1.1.128 2,2',3,3',4,4'-Hexachlorobiphenyl (PCB-128) .............................................. 1813
7.1.1.129 2,2',3,3',4,5-Hexachlorobiphenyl (PCB-129) .............................................. 1816
7.1.1.130 2,2',3,3',4,5'-Hexachlorobiphenyl (PCB-130) .............................................. 1818
7.1.1.131 2,2',3,3',4,6-Hexachlorobiphenyl (PCB-131) .............................................. 1820
7.1.1.132 2,2',3,3',4,6'-Hexachlorobiphenyl (PCB-132) .............................................. 1822
7.1.1.133 2,2',3,3',5,5'-Hexachlorobiphenyl (PCB-133) .............................................. 1824
7.1.1.134 2,2',3,3',5,6-Hexachlorobiphenyl (PCB-134) .............................................. 1826
7.1.1.135 2,2',3,3',5,6'-Hexachlorobiphenyl (PCB-135) .............................................. 1828
7.1.1.136 2,2',3,3',6,6'-Hexachlorobiphenyl (PCB-136) .............................................. 1830
7.1.1.137 2,2',3,4,4',5-Hexachlorobiphenyl (PCB-137) .............................................. 1833
7.1.1.138 2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138) .............................................. 1835
7.1.1.139 2,2',3,4,4',6-Hexachlorobiphenyl (PCB-139) .............................................. 1840
7.1.1.140 2,2',3,4,4',6'-Hexachlorobiphenyl (PCB-140) .............................................. 1842
7.1.1.141 2,2',3,4,5,5'-Hexachlorobiphenyl (PCB-141) .............................................. 1844
7.1.1.142 2,2',3,4,5,6-Hexachlorobiphenyl (PCB-142) .............................................. 1847
7.1.1.143 2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-143) .............................................. 1849
7.1.1.144 2,2',3,4,5',6-Hexachlorobiphenyl (PCB-144) .............................................. 1851
7.1.1.145 2,2',3,4,6,6'-Hexachlorobiphenyl (PCB-145) .............................................. 1853
7.1.1.146 2,2',3,4,5,5'-Hexachlorobiphenyl (PCB-146) .............................................. 1855
7.1.1.147 2,2',3,4,5,6-Hexachlorobiphenyl (PCB-147) .............................................. 1857
7.1.1.148 2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-148) .............................................. 1859
7.1.1.149 2,2',3,4',5',6'-Hexachlorobiphenyl (PCB-149) .............................................. 1861
7.1.1.150 2,2',3,4',6,6'-Hexachlorobiphenyl (PCB-150) ................................................ 1863
7.1.1.151 2,2',3,5,5',6'-Hexachlorobiphenyl (PCB-151) ................................................ 1865
7.1.1.152 2,2',3,5,6,6'-Hexachlorobiphenyl (PCB-152) ................................................ 1868
7.1.1.153 2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153) ................................................. 1870
7.1.1.154 2,2',4,4',5,6'-Hexachlorobiphenyl (PCB-154) ................................................ 1877
7.1.1.155 2,2',4,4',6,6'-Hexachlorobiphenyl (PCB-155) ................................................ 1879
7.1.1.156 2,3',4,4',5-Hexachlorobiphenyl (PCB-156) .................................................... 1883
7.1.1.157 2,3',4,4',5'-Hexachlorobiphenyl (PCB-157) .................................................... 1885
7.1.1.158 2,3',4,4',6-Hexachlorobiphenyl (PCB-158) ..................................................... 1887
7.1.1.159 2,3',4,5,5'-Hexachlorobiphenyl (PCB-159) .................................................... 1889
7.1.1.160 2,3',4,5,6-Hexachlorobiphenyl (PCB-160) ..................................................... 1891
7.1.1.161 2,3',4,5,5'-Hexachlorobiphenyl (PCB-161) ..................................................... 1893
7.1.1.162 2,3',4,5,5'-Hexachlorobiphenyl (PCB-162) ..................................................... 1895
7.1.1.163 2,3',4,5,6-Hexachlorobiphenyl (PCB-163) ..................................................... 1897
7.1.1.164 2,3',4,5',6-Hexachlorobiphenyl (PCB-164) ................................................... 1899
7.1.1.165 2,3',5,5',6-Hexachlorobiphenyl (PCB-165) .................................................... 1901
7.1.1.166 2,3',4,5,6-Hexachlorobiphenyl (PCB-166) ..................................................... 1903
7.1.1.167 2,3',4,4',5,5'-Hexachlorobiphenyl (PCB-167) ................................................ 1905
7.1.1.168 2,3',4,4',5,6-Hexachlorobiphenyl (PCB-168) ................................................ 1907
7.1.1.169 3,3',4,4',5,5'-Hexachlorobiphenyl (PCB-169) ................................................ 1909
7.1.1.170 2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB-170) .......................................... 1911
7.1.1.171 2,2',3,3',4,4',6-Heptachlorobiphenyl (PCB-171) .......................................... 1913
7.1.1.172 2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB-172) ......................................... 1915
7.1.1.173 2,2',3,3',4,5,6-Heptachlorobiphenyl (PCB-173) .......................................... 1917
7.1.1.174 2,2',3,3',4,5,6'-Heptachlorobiphenyl (PCB-174) ........................................ 1919
7.1.1.175 2,2',3,3',4,5',6-Heptachlorobiphenyl (PCB-175) ........................................ 1921
7.1.1.176 2,2',3,3',4,6,6'-Heptachlorobiphenyl (PCB-176) ........................................ 1923
7.1.1.177 2,2',3,3',4,5,6'-Heptachlorobiphenyl (PCB-177) ....................................... 1925
7.1.1.178 2,2',3,3',5,5,6'-Heptachlorobiphenyl (PCB-178) ....................................... 1927
7.1.1.179 2,2',3,3',5,5,6'-Heptachlorobiphenyl (PCB-179) ....................................... 1929
7.1.1.180 2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180) ...................................... 1931
7.1.1.181 2,2',3,4,4',5,6-Heptachlorobiphenyl (PCB-181) ...................................... 1935
7.1.1.182 2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-182) ...................................... 1937
7.1.1.183 2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-183) ...................................... 1939
7.1.1.184 2,2',3,4,4',6,6'-Heptachlorobiphenyl (PCB-184) ...................................... 1941
7.1.1.185 2,2',3,4,5,5,6'-Heptachlorobiphenyl (PCB-185) ...................................... 1943
7.1.1.186 2,2',3,4,5,6,6'-Heptachlorobiphenyl (PCB-186) ...................................... 1945
7.1.1.187 2,2',3,4,5,5,6'-Heptachlorobiphenyl (PCB-187) ...................................... 1947
7.1.1.188 2,2',3,4,5,5,6'-Heptachlorobiphenyl (PCB-188) ...................................... 1950
7.1.1.189 2,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189) ...................................... 1952
7.1.1.190 2,3',4,4',5,6-Heptachlorobiphenyl (PCB-190) ...................................... 1954
7.1.1.191 2,3',4,4',5,6-Heptachlorobiphenyl (PCB-191) ...................................... 1956
7.1.1.192 2,3',4,5,5,6-Heptachlorobiphenyl (PCB-192) ...................................... 1958
7.1.1.193 2,3',4,5,5,6-Heptachlorobiphenyl (PCB-193) ...................................... 1960
7.1.1.194 2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB-194) .................................. 1962
7.1.1.195 2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-195) .................................. 1965
7.1.1.196 2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-196) .................................. 1967
7.1.1.197 2,2',3,3',4,4',6,6'-Octachlorobiphenyl (PCB-197) .................................. 1969
7.1.1.198 2,2',3,3',4,5,5,6-Octachlorobiphenyl (PCB-198) .................................. 1971
7.1.1.199 2,2',3,3',4,5,5',6'-Octachlorobiphenyl (PCB-199) .................................. 1973
7.1.1.200 2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200) .................................. 1975
7.1.1.201 2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-201) .................................. 1977
7.1.1.202 2,2',3,3',5,5,6,6'-Octachlorobiphenyl (PCB-202) .................................. 1979
7.1.1.203 2,2',3,4,4',5,5,6-Octachlorobiphenyl (PCB-203) .................................. 1983
7.1.1.204 2,2',3,4,4',5,6,6'-Octachlorobiphenyl (PCB-204) ................................. 1985
7.1.1.205 2,3,3',4,4',5,5',6-Octachlorobiphenyl (PCB-205) ............................... 1987
7.1.1.206 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB-206) .......................... 1989
7.1.1.207 2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl (PCB-207) ......................... 1991
7.1.1.208 2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl (PCB-208) ......................... 1993
7.1.1.209 2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl (PCB-209) ..................... 1995

7.1.2 Isomer groups ................................................................. 1999
7.1.2.1 Monochlorobiphenyl ......................................................... 1999
7.1.2.2 Dichlorobiphenyl .......................................................... 2001
7.1.2.3 Trichlorobiphenyl .......................................................... 2003
7.1.2.4 Tetrachlorobiphenyl ......................................................... 2005
7.1.2.5 Pentachlorobiphenyl ......................................................... 2007
7.1.2.6 Hexachlorobiphenyl .......................................................... 2009
7.1.2.7 Heptachlorobiphenyl ......................................................... 2011
7.1.2.8 Octachlorobiphenyl .......................................................... 2013
7.1.2.9 Nonachlorobiphenyl ......................................................... 2014

7.1.3 Aroclor mixtures .............................................................. 2015
7.1.3.1 Aroclor 1016 ................................................................. 2015
7.1.3.2 Aroclor 1221 ................................................................. 2017
7.1.3.3 Aroclor 1232 ................................................................. 2019
7.1.3.4 Aroclor 1242 ................................................................. 2021
7.1.3.5 Aroclor 1248 ................................................................. 2024
7.1.3.6 Aroclor 1254 ................................................................. 2026
7.1.3.7 Aroclor 1260 ................................................................. 2030

7.2 Summary Tables and QSPR Plots ............................................. 2033
7.3 References ................................................................. 2047

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
7.1 LIST OF CHEMICALS AND DATA COMPILATIONS

7.1.1 PCB CONGENERS

7.1.1.0 Biphenyl

(See also Chapter 4, Polynuclear Aromatic Hydrocarbons [PAHs] and Related Aromatic Hydrocarbons)

Common Name: Biphenyl
Synonym: diphenyl, phenylbenzene
Chemical Name: biphenyl
CAS Registry No: 92-52-4
Molecular Formula: C₁₂H₁₀
Molecular Weight: 154.207
Melting Point (°C):
   68.93 (Lide 2003)
Boiling Point (°C):
   256.1 (Lide 2003)
Density (g/cm³ at 20°C):
   0.866 (20°C, Weast 1982–1983)
   1.04 (Lide 2003)
Molar Volume (cm³/mol):
   148.3 (20°C, calculated-density)
   184.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
   18.58 (Parks & Huffman 1931)
   18.66 (exptl., Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
   51.05 (Miller et al. 1984)
   54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
   0.371 (mp at 68.93°C)
   0.35 (Mackay et al. 1980, 1983; Shiu & Mackay 1986; Shiu et al. 1987)
   0.381 (calculated, $\Delta S_{\text{fus}} = 54$ J/mol K, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   5.94 (shake flask-UV, Andrews & Keefer 1949)
   7.48* (shake flask-UV, measured range 0.4–42.8°C, Bohon & Claussen 1951)
   3.87 (shake flask-UV, Sahyun 1966)
   7.08* (shake flask-UV, measured range 0–64.5°C, Wauchope & Getzen 1972)
   $R \ln x = -4520/(T/K) + 4.08 \times 10^{-4}[(T/K) - 298.15]^2 - 20.8 + 0.0273\times(T/K)$, temp range 24.6–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)
   7.45 (shake flask-GC, Eganhouse & Calder 1976)
   7.0 (shake flask-fluorescence, Mackay & Shiu 1977)
   8.50 (shake flask-nephelometry, Hollifield 1979)
   7.51 (shake flask-LSC, Banerjee et al. 1980)
   8.09 (TLC-RT correlation, Bruggeman et al. 1982)
   7.09 (recommended, Pearlman et al. 1984)
   7.05 (vapor saturation-UV, Akiyoshi et al. 1987)
   6.5 (29°C, shake flask-GC/FID; Stucki & Alexander 1987)
   7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)
Polychlorinated Biphenyls (PCBs)

9.96, 9.96, 9.96, 10.67 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)

7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)
\[ \log [S_i/(\text{mol/L})] = 1.872 - 973.4/(T/K) \] (supercooled liquid, Passivirta et al. 1999)
\[ \ln x = -1.5792 - 3669.26/(T/K) \] (temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)
104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)
133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)
1.30 (effusion method, measured range 4.0–34.5°C, Bright 1951)
\[ \log (P/mmHg) = 10.38 - 3799/(T/K) \] (temp range 4.0–34.5°C (Antoine eq., effusion Bright 1951)
0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)
1.273* (effusion method, measured range 15.05–40.55°C, Bradley & Cleasby 1953)
\[ \log (P/mmHg) = 11.282 - 4263/(T/K) \] (temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)
\[ \log (P/mmHg) = [-0.2185 \times 12910.0/(T/K)] + 8.218583 \] (temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)
1.41* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitaiagorodskii 1974)
\[ \log (P/mmHg) = 12.6789 - 4367.1/(T/K) \] (temp range 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitaiagorodskii 1974)
2040* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)
1.40 (HPLC-RT correlation, Swann et al. 1983)
3.35, 3.41 (P GC by GC-RT correlation, different GC columns, Bidleman 1984)
5.608 (supercooled liquid P L, converted from literature P S with ∆S fus Bidleman 1984)
\[ \log (P/kPa) = 6.36895 - 1997.558/(202.608 + t/°C) \] (temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)
\[ \log (P/Pa) = 14.840 - 4402.1/(T/K) \] (temp range 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
2.03 (supercooled liquid P L, GC-RI correlation, Burkhard et al. 1985b)
\[ \log (P/mmHg) = 7.24541 - 1998.725/(202.733 + w°C) \] (temp range 69–271°C (Antoine eq., Dean 1985, 1992)
5.61; 6.62 (supercooled liquid P L, quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)
2.43; 6.90 (selected P S, supercooled liq. P L, Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)
1.443; 1.23 (P S, interpolated-Antoine equations; Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 11.71929 - 4143.054/(T/K) \] (temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 28.5175 - 2114.5/(T/K) \] (temp range 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 6.37526 - 1794.8/(–74.85 + T/K) \] (temp range 390–563 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
5.10, 5.00 (supercooled P L, converted from literature P S with different ∆S fus values, Hinckley et al. 1990)
3.35 (P GC by GC-RT correlation, Hinckley et al. 1990)
0.422–2.54; 2.03–7.04 (quoted range of lit. P S values; lit. P L values, Delle Site 1997)
5.31; 2.02 (quoted supercooled liquid P L from Hinckley et al. 1990; converted to solid P S with fugacity ratio F, Passivirta et al. 1999)
\[ \log (P/Pa) = 11.05 - 3201/(T/K) \] (solid, Passivirta et al. 1999)
\[ \log (P/Pa) = 8.20 - 2228/(T/K) \] (supercooled liquid, Passivirta et al. 1999)
\[ \log (P/kPa) = 14.840 - 4402.1/(T/K) \] (temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
3.63; 0.822 (supercooled liquid P L, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
\[ \log (P/Pa) = -3265/(T/K) + 11.51; \Delta H_{vap} = -62.5 \text{ kJ·mol}^{-1} \] (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>41.34</td>
<td>batch stripping-GC</td>
<td>Mackay et al. 1979</td>
</tr>
<tr>
<td>30.4</td>
<td>batch stripping-GC</td>
<td>Mackay et al. 1980</td>
</tr>
<tr>
<td>11.55</td>
<td>gas stripping-GC</td>
<td>Warner et al. 1987</td>
</tr>
<tr>
<td>19.57</td>
<td>wetted-wall column-GC</td>
<td>Fendinger &amp; Glotfelty 1990</td>
</tr>
<tr>
<td>31.20</td>
<td>gas stripping-GC</td>
<td>Shiu &amp; Mackay 1997</td>
</tr>
<tr>
<td>log [H/(Pa m³/mol)] = 6.33 – 1255/(T/K)</td>
<td>(Passivirta et al. 1999)</td>
<td></td>
</tr>
</tbody>
</table>

Octanol/Water Partition Coefficient, log $K_{ow}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.16</td>
<td>shake flask-UV</td>
<td>Rogers &amp; Cammarata 1969</td>
</tr>
<tr>
<td>4.09</td>
<td>shake flask</td>
<td>Leo et al. 1971; Hansch &amp; Leo 1979</td>
</tr>
<tr>
<td>4.04</td>
<td>shake flask</td>
<td>Hansch et al. 1973</td>
</tr>
<tr>
<td>4.17, 4.09, 3.16, 4.04</td>
<td>(Neely et al. 1974; Hansch &amp; Leo 1979)</td>
<td></td>
</tr>
<tr>
<td>3.95</td>
<td>HPLC-$k'$ correlation</td>
<td>Rekker &amp; De Kort 1979</td>
</tr>
<tr>
<td>3.75</td>
<td>HPLC-RT correlation</td>
<td>Veith et al. 1979a</td>
</tr>
<tr>
<td>4.04</td>
<td>shake flask-HPLC</td>
<td>Banerjee et al. 1980</td>
</tr>
<tr>
<td>3.88</td>
<td>lit. average</td>
<td>Kenaga &amp; Goring 1980</td>
</tr>
<tr>
<td>4.10</td>
<td>(RP-TLC-$k'$ correlation</td>
<td>Bruggeman et al. 1982</td>
</tr>
<tr>
<td>4.08</td>
<td>(HPLC-$k'$ correlation, Hammers et al. 1982)</td>
<td></td>
</tr>
<tr>
<td>3.70</td>
<td>(HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)</td>
<td></td>
</tr>
<tr>
<td>3.16–4.09, 3.91</td>
<td>(shake flask, range, average, Eadsforth &amp; Moser, 1983)</td>
<td></td>
</tr>
<tr>
<td>3.91–4.15, 4.05</td>
<td>(HPLC, range, average, Eadsforth &amp; Moser 1983)</td>
<td></td>
</tr>
<tr>
<td>4.03</td>
<td>(HPLC-$k'$ correlation, Hafkenscheid &amp; Tomlinson 1983)</td>
<td></td>
</tr>
<tr>
<td>3.93</td>
<td>(HPLC correlation; Harnisch et al. 1983)</td>
<td></td>
</tr>
<tr>
<td>3.76</td>
<td>(generator column-GC/ECD, Miller et al. 1984,1985)</td>
<td></td>
</tr>
<tr>
<td>3.89</td>
<td>(generator column-HPLC, Woodburn et al. 1984)</td>
<td></td>
</tr>
<tr>
<td>3.79</td>
<td>(RP-HPLC-RT correlation, Rapaport &amp; Eisenreich 1984)</td>
<td></td>
</tr>
<tr>
<td>4.11–4.13</td>
<td>(HPLC-RV correlation, quoted exp., Garst 1984)</td>
<td></td>
</tr>
<tr>
<td>4.10</td>
<td>(HPLC-RV correlation, Garst &amp; Wilson 1984)</td>
<td></td>
</tr>
<tr>
<td>4.05</td>
<td>(HPLC-RT correlation, Eadsforth 1986)</td>
<td></td>
</tr>
<tr>
<td>3.81</td>
<td>(shake flask-GC, Menges &amp; Armstrong 1986)</td>
<td></td>
</tr>
<tr>
<td>4.13</td>
<td>(HPLC-RT correlation, Wang et al. 1991)</td>
<td></td>
</tr>
<tr>
<td>3.63</td>
<td>(HPLC-$k'$ correlation; De Kock &amp; Lord 1987)</td>
<td></td>
</tr>
<tr>
<td>3.89</td>
<td>(generator column-GC, Doucette &amp; Andren 1987,1988)</td>
<td></td>
</tr>
<tr>
<td>4.14, 4.06, 4.00, 3.94</td>
<td>(RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
<td></td>
</tr>
<tr>
<td>3.69</td>
<td>(HPLC-RT correlation, Doucette &amp; Andren 1988)</td>
<td></td>
</tr>
<tr>
<td>3.75</td>
<td>(HPLC-RT correlation, Sherblom &amp; Eganhouse 1988)</td>
<td></td>
</tr>
<tr>
<td>4.008; 4.10</td>
<td>(slow stirring-GC; calculated-$\pi$ const., De Bruijn et al. 1989; De Bruijn &amp; Hermens 1990)</td>
<td></td>
</tr>
<tr>
<td>3.98</td>
<td>(recommended, Sangster 1989, 1993)</td>
<td></td>
</tr>
<tr>
<td>4.29</td>
<td>(dual-mode centrifugal partition chromatography, Gluck &amp; Martin 1990)</td>
<td></td>
</tr>
<tr>
<td>4.26</td>
<td>(HPLC-$k'$ correlation, Noegrohati &amp; Hammers 1992)</td>
<td></td>
</tr>
<tr>
<td>4.01</td>
<td>(recommended, Hansch et al. 1995)</td>
<td></td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.92, 6.09; 6.09</td>
<td>(0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)</td>
<td></td>
</tr>
<tr>
<td>6.15</td>
<td>(calculated-$S_\text{oct}$ and vapor pressure $P$, Abraham et al. 2001)</td>
<td></td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.64</td>
<td>(trout, calculated-$k_1/k_2$, Neely et al. 1974)</td>
<td></td>
</tr>
<tr>
<td>3.12</td>
<td>(rainbow trout, Veith et al. 1979; Veith &amp; Kosian 1983)</td>
<td></td>
</tr>
<tr>
<td>2.53</td>
<td>(fish, flowing water, Kenaga &amp; Goring 1980; Kenaga 1980)</td>
<td></td>
</tr>
<tr>
<td>2.73, 2.45, 3.41</td>
<td>(algae, fish, activated sludge, Freitag et al. 1985)</td>
<td></td>
</tr>
</tbody>
</table>
Sorption Partition Coefficient, $\log K_{OC}$:

- 3.15 (soil, Kenaga 1980)
- 3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)
- 5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)
- 3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)
- 3.40 (calculated, soil, Chou & Griffin 1986)
- 4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
- 3.03, 3.12 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average values, Delle Site 2001)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: $t_{1/2} = 7.52$ d evaporation from water depth of 1 m (Mackay & Leinonen 1975)
- rate of volatilization $k = 0.92$ g m$^{-2}$ h$^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
- Photolysis: $k = 5.1 \times 10^{-4}$ h$^{-1}$ to $7.4 \times 10^{-3}$ h$^{-1}$ with $H_2O_2$ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);
- photodegradation $k = 5.1 \times 10^{-4}$ min$^{-1}$ and $t_{1/2} = 22.61$ h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (8.06 \pm 0.77) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with an estimated lifetime of $\sim$3 d, and $k_{O3} < 2.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294 $\pm$ 1 K (relative rate method, Atkinson et al. 1984)
  - $k_{OH} = (8.5 \pm 0.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1985)
  - $k_{OH} = (7 \pm 2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1985)
  - $k_{OH}(calc) = 7.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = (5.8 - 8.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
  - $k_{OH}(calc) = 7.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (SAR structure-activity relationship, Atkinson 1987b)
  - $k_{O3} < 2 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH} = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{NO3} < 2.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with N$_2$O$_5$ at room temp (Atkinson & Aschmann 1988)
  - $k_{OH}* = 7.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
  - $k_{OH}(calc) = 6.44 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)
  - $k_{OH}(exptl) = 7.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(calc) = 6.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972)
- $k = 109$ yr$^{-1}$ in the water column and $k = 1090$ yr$^{-1}$ in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981)
- $k = 9.3-9.8$ nmol L$^{-1}$ d$^{-1}$ with an initial biphenyl concentration of 4.4-4.7 $\mu$mol/L, and $k = 3.2$ nmol L$^{-1}$ d$^{-1}$ with initial concentration of 2.9 $\mu$mol/L, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
- $t_{1/2} = 1.5$ d, estimated by using water die-away test (Bailey et al. 1983)
- $t_{1/2}(aq.$ aerobic$) = 36-168$ h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
- $t_{1/2}(aq.$ anaerobic$) = 144-672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)⁻¹, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

- k₁ = 6.79 h⁻¹; k₂ = 0.0155 h⁻¹ (trout muscle, Neely et al. 1974; Neely 1979)
- k₁ = 6.8 h⁻¹; 1/k₂ = 65 h (trout, quoted, Hawker & Connell 1985)
- log k₁ = 2.21 d⁻¹; log 1/k₂ = 0.43 d (fish, Connell & Hawker 1988)
- log k₂ = −0.43 d⁻¹ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

- Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of ~1 × 10⁶ molecule/cm³ (Atkinson et al. 1984); estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical concn of 5 × 10⁶ cm⁻³ (Atkinson & Aschmann 1985); calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);
- t₀₁ = 7.8–110 h, based on photooxidation half-life in air (Howard et al. 1991);
- tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for biphenyl (Kwok et al. 1995).

- Surface water: t₀₁ ~1.5 d in river water (Bailey et al. 1983);
- t₀₁ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
- photolysis t₀₁ = 19.18 min in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

- Groundwater: t₀₁ = 72–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
- Sediment:
- Soil: t₀₁ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
- Biota: estimated t₀₁ = 29 h from fish in simulated ecosystem (Neely 1980).

### TABLE 7.1.1.0.1

<table>
<thead>
<tr>
<th>Reported aqueous solubilities of biphenyl at various temperatures:</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bohon &amp; Claussen 1951</strong></td>
</tr>
<tr>
<td>shake flask-UV</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>0.40</td>
</tr>
<tr>
<td>2.4</td>
</tr>
<tr>
<td>5.2</td>
</tr>
<tr>
<td>7.6</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>12.6</td>
</tr>
<tr>
<td>14.9</td>
</tr>
<tr>
<td>15.9</td>
</tr>
<tr>
<td>25</td>
</tr>
<tr>
<td>25.6</td>
</tr>
<tr>
<td>30.1</td>
</tr>
<tr>
<td>30.4</td>
</tr>
<tr>
<td>33.3</td>
</tr>
<tr>
<td>34.9</td>
</tr>
<tr>
<td>36</td>
</tr>
<tr>
<td>42.8</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>
Polychlorinated Biphenyls (PCBs)

TABLE 7.1.1.0.1 (Continued)

<table>
<thead>
<tr>
<th>Bohon &amp; Claussen 1951</th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Shaw 1989</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-UV</td>
<td>shake flask-UV</td>
<td>IUPAC recommended</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g}\cdot\text{m}^{-3} )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>for supercooled liquid: ( \Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) ) = &amp; ( 47.5 ) &amp; ( 18.7 ) &amp; ( \ln x ) &amp; mole fraction &amp; ( 50.1 ) &amp; ( 20.6 ) &amp; ( \Delta H_{\text{fus}} ) &amp; ( 18.9 \pm 0.50 ) &amp; ( 50.1 ) &amp; ( 20.6 ) ( \times 10^2 \times b ) &amp; ( 2.73 \pm 0.12 ) &amp; ( 20.8 \pm 0.4 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 275 K &amp; 7.03 &amp; 50.1 &amp; 21.6 &amp; ( \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) ) &amp; 50.1 &amp; 21.8 &amp; ( c ) &amp; 20.8 &amp; 0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>280 K &amp; 10.13 &amp; 50.2 &amp; 21.8 &amp; &amp; 50.2 &amp; 21.8 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>290 K &amp; 12.55 &amp; 54.7 &amp; 28.3 &amp; &amp; 54.7 &amp; 28.8 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>295 K &amp; 13.43 &amp; 54.7 &amp; 28.3 &amp; &amp; 54.7 &amp; 28.8 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>300 K &amp; 15.02 &amp; 54.7 &amp; 28.3 &amp; &amp; 54.7 &amp; 28.8 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>305 K &amp; 18.58 &amp; 59.2 &amp; 36.4 &amp; &amp; 59.2 &amp; 36.4 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>310 K &amp; 21.42 &amp; 59.2 &amp; 36.4 &amp; &amp; 59.2 &amp; 36.4 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>315 K &amp; 21.09 &amp; 60.5 &amp; 40.4 &amp; &amp; 60.5 &amp; 40.4 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>&amp; &amp; 64.5 &amp; 43.7, 44.7 &amp; &amp; 64.5 &amp; 46.5 &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>&amp; &amp; &amp; &amp; &amp; &amp; &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) ) = 18.91 &amp; &amp; &amp; &amp; &amp; &amp; &amp; &amp; &amp;</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Empirical temperature dependence equations:
Wauchope & Getzen (1972): \( R \cdot \ln x = –[H_{\text{fus}}/(T/K)] + (0.000408)\left[(T/K) – 291.15\right]^2 -c + b\times(T/K) \) (1)

FIGURE 7.1.1.0.1 Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for biphenyl.
TABLE 7.1.1.0.2
Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

log \( P = A - \frac{B}{(T/K)} \) \hspace{1cm} (1) \hspace{1cm} ln \( P = A - \frac{B}{(T/K)} \) \hspace{1cm} (1a)

log \( P = A - \frac{B}{(C + t/°C)} \) \hspace{1cm} (2) \hspace{1cm} ln \( P = A - \frac{B}{(C + t/°C)} \) \hspace{1cm} (2a)

log \( P = A - \frac{B}{(C + T/K)} \) \hspace{1cm} (3)

log \( P = A - \frac{B}{(T/K)} - C\cdot\log{(T/K)} \) \hspace{1cm} (4)

log \( P = A - \frac{B}{(T/K)} - \frac{C}{(T/K)^2} \) \hspace{1cm} (5)

1.

<table>
<thead>
<tr>
<th>Chipman &amp; Peltier 1929</th>
<th>Stull 1947 summary of literature data</th>
<th>Bright 1951 eq. 1 P/mmHg</th>
<th>Bradley &amp; Cleasby 1953 eq. 1 P/mmHg</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
</tr>
<tr>
<td>162.5</td>
<td>7933</td>
<td>70.6</td>
<td>133.3</td>
</tr>
<tr>
<td>172.3</td>
<td>10959</td>
<td>101.8</td>
<td>666.6</td>
</tr>
<tr>
<td>177.7</td>
<td>12799</td>
<td>117.0</td>
<td>1333</td>
</tr>
<tr>
<td>183.5</td>
<td>15705</td>
<td>134.2</td>
<td>2666</td>
</tr>
<tr>
<td>191.6</td>
<td>19972</td>
<td>152.5</td>
<td>5333</td>
</tr>
<tr>
<td>198.75</td>
<td>24691</td>
<td>165.2</td>
<td>7999</td>
</tr>
<tr>
<td>293.8</td>
<td>28504</td>
<td>180.7</td>
<td>13332</td>
</tr>
<tr>
<td>211.25</td>
<td>34677</td>
<td>204.2</td>
<td>26664</td>
</tr>
<tr>
<td>220.05</td>
<td>43756</td>
<td>229.4</td>
<td>53329</td>
</tr>
<tr>
<td>229.8</td>
<td>56329</td>
<td>254.0</td>
<td>101325</td>
</tr>
<tr>
<td>238.2</td>
<td>68901</td>
<td></td>
<td></td>
</tr>
<tr>
<td>247.7</td>
<td>85580</td>
<td></td>
<td></td>
</tr>
<tr>
<td>253.7</td>
<td>98019</td>
<td></td>
<td></td>
</tr>
<tr>
<td>255.2</td>
<td>101178</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

bp/°C \(266.25\)

ΔH\textsubscript{v}/(kJ mol\textsuperscript{-1}) = 44.99

at bp

eq. 5 P/mmHg

A \(7.0220\)
B \(1723\)
C \(245700\)

temp range 162–322°C
TABLE 7.1.0.2 (Continued)

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
</tr>
<tr>
<td>24.9 1.433</td>
<td>123.0 2040</td>
<td>5.2 0.106</td>
<td>69.20 104</td>
<td></td>
</tr>
<tr>
<td>31.75 2.976</td>
<td>143.81 4773</td>
<td>14.9 0.361</td>
<td>93.3 413</td>
<td></td>
</tr>
<tr>
<td>33.7 3.734</td>
<td>164.69 9962</td>
<td>24.7 1.15</td>
<td>148.7 4833</td>
<td></td>
</tr>
<tr>
<td>35.5 4.538</td>
<td>181.28 1647</td>
<td>eq. 1 P/Pa</td>
<td>160.0 7239</td>
<td></td>
</tr>
<tr>
<td>37.6 5.726</td>
<td>200.87 28599</td>
<td>A 14.840</td>
<td>171.1 10548</td>
<td></td>
</tr>
<tr>
<td>39.57 6.913</td>
<td>223.66 51518</td>
<td>B 4402.1</td>
<td>182.2 15031</td>
<td></td>
</tr>
<tr>
<td>41.52 8.26</td>
<td>245.65 86254</td>
<td></td>
<td>193.3 21098</td>
<td></td>
</tr>
<tr>
<td>43.48 10.26</td>
<td>257.91 111343</td>
<td></td>
<td>204.4 28958</td>
<td></td>
</tr>
<tr>
<td>45.45 12.35</td>
<td>274.09 154493</td>
<td></td>
<td>215.6 39093</td>
<td></td>
</tr>
<tr>
<td>47.4 15.49</td>
<td>296.14 235345</td>
<td></td>
<td>226.7 51986</td>
<td></td>
</tr>
<tr>
<td>50.0 19.46</td>
<td>315.19 329300</td>
<td></td>
<td>237.8 68051</td>
<td></td>
</tr>
<tr>
<td></td>
<td>327.55 400175</td>
<td></td>
<td>248.9 88252</td>
<td></td>
</tr>
<tr>
<td>eq. 1 P/mmHg A</td>
<td>12.6789</td>
<td></td>
<td>255.3 101353</td>
<td></td>
</tr>
<tr>
<td>B 4367.436</td>
<td></td>
<td></td>
<td>6.36895</td>
<td></td>
</tr>
<tr>
<td>for temp range 24.9–50°C</td>
<td></td>
<td></td>
<td>1997.558</td>
<td></td>
</tr>
</tbody>
</table>

Sharma & Palmer 1974

gas saturation-GC

<table>
<thead>
<tr>
<th>t/°C P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>53.05 16.0</td>
</tr>
<tr>
<td>61.05 34.66</td>
</tr>
<tr>
<td>71.95 92.0</td>
</tr>
<tr>
<td>81.05 220.0</td>
</tr>
</tbody>
</table>

FIGURE 7.1.0.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.
7.1.1.1 2-Chlorobiphenyl (PCB-1)

Common Name: 2-Chlorobiphenyl
Synonym: PCB-1, o-chlorobiphenyl, 2-chloro-1,1′-biphenyl
Chemical Name: 2-chlorobiphenyl
CAS Registry No: 2051-60-7
Molecular Formula: C_{12}H_{9}Cl
Molecular Weight: 188.652

Boiling Point (°C): 274 (Weast 1972–73, 1982–83; Lide 2003)
Density (g/cm³ at 20°C): 0.9837

Molar Volume (cm³/mol):
- 205.5 (calculated-Le Bas method at normal boiling point)
- 172.9 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):
- 57.8 (Geidarov et al. 1975)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
- 72.3 (Geidarov et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 14.52 (Geidarov et al. 1975)
- 15.3 (differential scanning calorimetry, Miller et al. 1984)
- 14.54 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):
- 47.66 (Geidarov et al. 1975)
- 50.21 (Miller et al. 1984)

Fugacity Ratio at 25°C, F (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 1.60 (Webb 1970)
- 0.90 (Hoover 1971)
- 5.90 (shake flask-GC/ECD, Wallnöfer et al. 1973)
- 4.13 (generator column-GC/ECD, Weil et al. 1974)
- 5.08 (supercooled liquid S_L, shake flask-GC/ECD, Chiou et al. 1983)
- 5.06 (generator column-GC/ECD, Miller et al. 1984,1985)
- 4.13, 4.74, 14.0, 4.13 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmider 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 133.3* (89.3°C, summary of literature data, temp range 89.3–267.5°C, Stull 1947)
- log (P/mmHg) = (8.306 ± 0.087) – (3018 ± 45)/(T/K), temp range: 410–510 K (static method-quartz manometer measurements, Geidarov et al. 1975)
- 1.84 (supercooled liquid P_L, extrapolated Antoine eq., Weast 1976–77)
- 1.12 (Neely 1981,1983)
- 0.605; 0.159; 0.367* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from expctl. derived Antoine eq., measured range 33–110°C, Ferro et al. 1983)
Polychlorinated Biphenyls (PCBs)

\[
\log (P/L/kPa) = -3893/(T/K) + 9.99; \text{ temp range: 33–77°C (Knudsen effusion data, Ferro et al. 1983)}
\]

\[
\log (P/L/kPa) = -4406/(T/K) + 10.98; \text{ temp range: 64–110°C (torsion effusion data, liquid, Ferro et al. 1983)}
\]

\[
\log (P/L/kPa) = -(4149 \pm 230)/(T/K) + (10.48 \pm 0.50); \text{ temp range: 33–110°C (torsion-Knudsen effusion data, Ferro et al. 1983)}
\]

1.096, 1.456 (PGC by GC-RT correlation, different stationary phases, Bidleman 1984)

1.892, 2.56 (supercooled liquid P_L from P_GC, GC-RT correlation, different stationary phases, Bidleman 1984)

0.755 (GC-RI correlation, Burkhard et al. 1985a)

0.926 (GC-RI correlation, supercooled liquid P_L, Burkhard et al. 1985b)

2.20 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)

1.096 (P_GC by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)

\[
\log (P/L/Pa) = -3366/(T/K) + 11.57 \text{ (GC-RT correlation, Falconer & Bidleman 1994)}
\]

0.27–2.70; 0.367–2.56 (literature P_S range; literature supercooled liquid P_L range, Delle Site 1997)

\[
\log (P/kPa) = 9.99 – 3893/(T/K); \text{ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

28.9 (calculated-P/C, Burkhard et al. 1985b)

70.1 (calculated-P/C, Shiu & Mackay 1986)

74.6 (Dow Chemical, Neely 1982)

30.18 (calculated-QSPR, Dunnivant et al. 1992)

5.13, 8.32, 13.17, 20.43 ± 0.52, 29.3 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)

\[
K_{AW} = \exp\left[-(42.7/JK^{-1}mol^{-1}/RT) + (0.104/JK^{-1}mol^{-1}K^{-1}/R)\right]; \text{ where } R = 8.314 JK^{-1}mol^{-1} \text{ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)}
\]

\[
\ln K_{AW} = -\Delta H_r/RT + \Delta S_r/R; \text{ R is the ideal gas constant, } \Delta H_r = 43 \pm 6 \text{ kJ/mol, } \Delta S_r = 0.10 \pm \text{ 0.02 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004)}
\]

Octanol/Water Partition Coefficient, log K_{ow}:

4.54 (shake flask-GC, Tulp & Hutzinger 1978)

4.80 (Hansch & Leo 1979)

4.35 (HPLC-RT correlation, Veith et al. 1979)

4.10 (HPLC-RT correlation, McDuffie 1981)

4.59 ± 0.1; 4.56 (shake flask-GC; RP-TLC-k′ correlation, Bruggeman et al. 1982)

3.75 (HPLC-RT correlation, Woodburn 1982)

4.51 (shake flask-GC, Chiu et al. 1983)

4.50 (generator column-GC, Miller et al. 1984, 1985)

4.38 (generator column-HPLC, Woodburn et al. 1984)

3.90, 4.60 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

4.44 (HPLC-RP/MS correlation, Burkhard & Kuehl 1986)

4.38 (generator column-GC/ECD, Doucette & Andren 1987)

4.33, 4.39, 4.53, 4.43 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

3.92 (HPLC-RT correlation, Doucette & Andren 1988)

4.531 ± 0.029 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)

4.52 (recommended, Sangster 1989, 1993)

4.68 (HPLC-k′ correlation, Noegrohati & Hammers 1992)

4.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa} or as indicated:

7.54, 6.65 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)

6.04 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:

- 3.50 (Woodburn silt loam soil, batch equilibrium isotherm-GC/ECD, Chiou et al. 1983)
- 4.35 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 3.47 (calculated, soil, Chou & Griffin 1986)
- 2.59 (Borden soil 0.29% OC, Hu et al. 1995)

Sorption Partition Coefficient, log $K_{OM}$:

- 3.23 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- **Volatilization:**
  - $k$ (calc) = $3.7 \times 10^{-4}$ d$^{-1}$ and with $t_{1/2}$ = 18 yr, calculated sunlight photolysis rate constant in surface water at 40°N (Dulin et al. 1986)
  - $k$ (calc) = 3.0 h$^{-1}$ maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)
  - $t_{1/2}$ = 31 d under sunlight in water (Mansour & Feicht 1994)
  - $k = 0.081$ min$^{-1}$ at pH 3, $k = 0.045$ min$^{-1}$ at pH 7 and $k = 0.035$ min$^{-1}$ at pH 10 with half-lives of 9, 15 and 20 min, respectively, in aqueous solutions when irradiated by UVA-340 light tubes in the presence of $25 \mu$g/mL of TiO$_2$;
  - $k = (0.043-0.045)$ min$^{-1}$ with $t_{1/2}$ = 15–16 min, $k = (0.082–0.091)$ min$^{-1}$ with $t_{1/2}$ = 8 min, and $k = (0.21–0.29)$ min$^{-1}$ with $t_{1/2}$ = 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively;
  - $k = (0.043-0.044)$ min$^{-1}$ with $t_{1/2}$ = 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of $100 \mu$g/mL TiO$_2$;
  - $k = (0.030–0.055)$ min$^{-1}$ with $t_{1/2}$ = 13–22 min in St. Lawrence River water containing $3 \mu$g/mL of total PCB irradiated by sunlight in the presence of $100 \mu$g/mL TiO$_2$ (Huang et al. 1996).

- **Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (2.9 \pm 0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K with estimated atmospheric lifetime of ~8 d (relative rate method, Atkinson & Aschmann 1985)
  - $k_{OH} = 1.6 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ to the C$_6$H$_4$Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ to ring A, and $k_{OH} = 2.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)
  - $k_{OH}$(calc) = $(2.8 – 5.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}$(exptl) = $(3.1 – 4.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987);
  - $k_{OH}(calc) = 2.82 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (Atkinson 1989)
  - $k_{OH}$(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(calc) = (3.2 – 4.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

- **Hydrolysis:**
  - Biodegradation: $t_{1/2}$ = 100 h biodegradation by bacteria (Wong & Kaiser 1975);
  - within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);
  - $k = 63 $yr$^{-1}$ microbial degradation pseudo first-order rate constant of in the water column and $k = 630 $yr$^{-1}$ in the sediment (Wong & Kaiser 1975; quoted, Neely 1981);
  - $k = 4.1 $nmol L$^{-1}$ d$^{-1}$ biodegradation rate in water from Port Valdez with an initial concn of 1.5 µmol/L (data of Aug. 1977, Reichardt et al. 1981) and $k = 1.2 $nmol L$^{-1}$ d$^{-1}$ with initial concn of 4.5 µmol/L (data of Aug. 1978, Reichardt et al. 1981); and $t_{1/2}$ = 2–3.5 d, an initial concn of 1–100 µg/L by river dieaway test (Bailey et al. 1983)
  - $k = 1.10 $µg mL$^{-1}$ d$^{-1}$, the degradation rate at 30 µg mL$^{-1}$, under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

- **Biotransformation:**
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~8 d due to reaction with the OH radical for a 24-h average OH radical concn of 5 × 10^9 cm^-3 (Atkinson & Aschmann 1985);

- calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);
- photolysis $t_{1/2}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);
- tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);
- tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 1.4$ d in Lake Michigan (Neely 1983);
- photolysis $t_{1/2}$ = 18 yr in surface water at 40° L in summer (Dulin et al. 1986);
- photolysis $t_{1/2} = 31$ d under sunlight (Mansour & Feicht 1994);
- half-lives in aqueous solutions with initial concn of 265 ng/mL, $t_{1/2} = 9$ min at pH 3, $t_{1/2} = 15$ min at pH 7 and $t_{1/2} = 20$ min at pH 10 when irradiated by UVA-340 light tubes (simulated sun light) in the presence of 25 µg/mL TiO_2; half-lives of 15–16 min, 8 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; half-lives of 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{1/2} = 13–22$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

### TABLE 7.1.1.1.1

Reported vapor pressures of 2-chlorobiphenyl (PCB-1) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Geidarov et al. 1975</th>
<th>Ferro et al. 1983</th>
</tr>
</thead>
<tbody>
<tr>
<td>compiled literature data</td>
<td>static-quartz manometer</td>
<td>torsion effusion</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>89.3</td>
<td>133.3</td>
<td>50</td>
</tr>
<tr>
<td>109.8</td>
<td>666.7</td>
<td>54</td>
</tr>
<tr>
<td>134.7</td>
<td>1333</td>
<td>59</td>
</tr>
<tr>
<td>151.2</td>
<td>2666</td>
<td>63</td>
</tr>
<tr>
<td>169.9</td>
<td>5333</td>
<td>range: 137–267°C</td>
</tr>
<tr>
<td>182.1</td>
<td>7999</td>
<td></td>
</tr>
<tr>
<td>197.0</td>
<td>13333</td>
<td>mp/°C</td>
</tr>
<tr>
<td>219.6</td>
<td>26664</td>
<td>bp/°C</td>
</tr>
<tr>
<td>243.8</td>
<td>53329</td>
<td></td>
</tr>
<tr>
<td>267.5</td>
<td>101325</td>
<td>$\Delta H_v/(kJ mol^{-1}) = 57.78$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\Delta H_{fus}/(kJ mol^{-1}) = 14.52$</td>
</tr>
</tbody>
</table>

(Continued)
### TABLE 7.1.1.1.1 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>mp/°C</td>
<td>34.0</td>
<td>mp/°C</td>
<td>86</td>
<td>mp/°C</td>
<td>28</td>
<td>mp/°C</td>
<td>206</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.762</td>
<td></td>
<td>0.762</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.50</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.52</td>
<td></td>
<td>1.52</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.30</td>
<td></td>
<td>2.30</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.05</td>
<td></td>
<td>3.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.81</td>
<td></td>
<td>3.81</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4.57</td>
<td></td>
<td>4.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6.10</td>
<td></td>
<td>6.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>10.98</td>
<td></td>
<td>10.98</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4406</td>
<td></td>
<td>4406</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.46</td>
<td></td>
<td>3.46</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.17</td>
<td></td>
<td>5.17</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6.10</td>
<td></td>
<td>6.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>9.69</td>
<td></td>
<td>9.69</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>10.48</td>
<td></td>
<td>10.48</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4149</td>
<td></td>
<td>4149</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>33–86°C</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>64–110°C</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### FIGURE 7.1.1.1.1 Logarithm of vapor pressure and Henry’s law constant versus reciprocal temperature for 2-chlorobiphenyl (PCB-1).
Common Name: 3-Chlorobiphenyl
Synonym: PCB-2, m-chlorobiphenyl, 3-chloro-1,1′-biphenyl
Chemical Name: 3-chlorobiphenyl
CAS Registry No: 2051-61-8
Molecular Formula: C_{12}H_9Cl
Molecular Weight: 188.652
Melting Point (°C):
16 (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
284.5 (Lide 2003)
Density (g/cm³ at 20°C): 0.9837
Molar Volume (cm³/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
15.31 (Miller et al. 1984)
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 1.0 (mp at 16°C)
Water Solubility (g/m³ or mg/L at 25°C):
3.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
1.30 (generator column-GC/ECD, Weil et al. 1974)
0.56, 0.82, 0.88, 0.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.63 (generator column-HPLC/UV, Billington et al. 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.723 (extrapolated P_{L}, Antoine eq., Weast 1972–73)
0.711; 4.01; 0.362* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptrl. derived Antoine eq., measured range 37–129°C, Ferro et al. 1983)
\log (P_{L}/kPa) = −3458/(T/K) + 8.45; temp range: 37–86°C (Knudsen effusion data, liquid, Ferro et al. 1983)
\log (P_{L}/kPa) = −3371/(T/K) + 8.91; temp range: 68–129°C (torsion effusion data, liquid, Ferro et al. 1983)
\log (P_{L}/kPa) = −(3614 ± 188)/(T/K) + (8.68 ± 0.47); temp range: 37–129°C (torsion-Knudsen effusion data, Ferro et al. 1983)
0.98, 1.01 (supercooled P_{L}, GC-RT correlation with different stationary phases, Bidleman 1984)
0.366 (GC-RI correlation, Burkhard et al. 1985a)
0.362 (liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)
0.997 (liquid P_{L}, GC-RT correlation, Foreman & Bidleman 1985)
\log (P_{L}/Pa) = −3476/(T/K) + 11.65 (liquid P_{L}, GC-RT correlation, Falconer & Bidleman 1994)
0.220–1.01 (quoted lit. range, Delle Site 1997)
\log (P/Pa) = 11.64178 − 3514.98/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
Henry’s Law Constant (Pa m³/mol at 25°C):
14.49 (calculated-P/C, Burkhard et al. 1985b)
75.55 (calculated-P/C, Shiu & Mackay 1986)
62.11 (Dow Chemical, Neely 1982)
27.78 (calculated-QSAR, Dunnivant et al. 1992)
\[
\ln K_{\text{AW}} = -\Delta H_{\text{f}/R} + \Delta S_{\text{f}/R} \; R \text{ is the ideal gas constant, } \Delta H_{\text{f}} = 54 \pm 3 \text{ kJ/mol, } \Delta S_{\text{f}} = 0.14 \pm 0.01 \text{ kJ/mol-K} \\
(Bamford et al. 2002) \text{—see Comment by Goss et al. 2004}
\]

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
- 4.54 (shake flask-GC/ECD, Tulp & Hutzinger 1978)
- 4.35 (HPLC-RT correlation, Veith et al. 1979)
- 4.80 (Hansch & Leo 1979)
- 4.71 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
- 4.72 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
- 4.35 (HPLC-RT correlation, Woodburn 1982)
- 4.58 (generator column-HPLC, Woodburn et al. 1984)
- 3.75 (HPLC-RT correlation, Woodburn et al. 1984)
- 4.60 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 4.60 (selected, Shiu & Mackay 1986)
- 4.58 (generator column-GC/ECD, Doucette & Andren 1987)
- 4.65 (RP-HPLC-k’ correlation, Brodsky & Ballschmitter 1988)
- 4.58 (recommended, Sangster 1989, 1993)
- 4.72 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
- 4.58 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\) at 25°C or as indicated:
- 7.86, 6.99 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 6.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log \(B_{\text{CF}}\):

Sorption Partition Coefficient, log \(K_{\text{OC}}\):
- 4.42 (suspended particulate matter, calculated-\(K_{\text{OW}}\), Burkhard 1984)
- 3.62 (calculated-S, soil, Chou & Griffin 1986)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{\frac{1}{2}}\):

Volatilization:

Photolysis:
\[t_{\frac{1}{2}} = 45 \text{ d under sunlight in water (Mansour & Feicht 1994)}\]
\[k(\text{calc}) = 0.5 \text{ h}^{-1}, \text{maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)}\]
\[k = (0.03-0.045) \text{ min}^{-1} \text{ with } t_{\frac{1}{2}} = 15-19 \text{ min, } k = (0.069-0.085) \text{ min}^{-1} \text{ with } t_{\frac{1}{2}} = 8-10 \text{ min, and} \]
\[k = (0.18-0.23) \text{ min}^{-1} \text{ with } t_{\frac{1}{2}} = 3-4 \text{ min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 } \mu \text{g/mL TiO}_2, \text{respectively; rate constant of } k = (0.027-0.042) \text{ min}^{-1} \text{ with } t_{\frac{1}{2}} = 16-26 \text{ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 } \mu \text{g/mL TiO}_2; \]
\[k = (0.033-0.036) \text{ min}^{-1} \text{ with } t_{\frac{1}{2}} = 19-21 \text{ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 } \mu \text{g/mL TiO}_2 (Huang et al. 1996).\]

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO}_3}\) with NO\(_3\) radical and \(k_{\text{O}_3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:
\[k_{\text{OH}} = (5.4 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \pm 1 \text{ K, with an estimated atmospheric lifetime of } \sim 4 \text{ d (relative rate method, Atkinson & Aschmann 1985)}\]
\[k_{\text{OH}} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ to the } C_6H_4Cl \text{ ring (ring B), } k_{\text{OH}} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ to ring A, and } k_{\text{OH}} = 5.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (observed ring A + ring B) with a calculated tropospheric lifetime of } 5-11 \text{ d (Atkinson 1987)}\]
\[k_{\text{OH}}(\text{calc}) = (2.8-5.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{OH}}(\text{exptl}) = (3.1-4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be } 5-11 \text{ d (Atkinson 1987)}\]
\[k_{\text{OH}} = 5.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K (Atkinson 1989)}\]
Polychlorinated Biphenyls (PCBs)

$\text{k}_{\text{OH}}(\text{exptl}) = (2.8 - 5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $\text{k}_{\text{OH}}(\text{calc}) = (3.2 - 4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

**Hydrolysis:**
Biodegradation: $t_{1/2} = 7$ h by Alcaligenes sp. strain Y-42 from lake sediments (Furukawa & Matsumara 1976; selected, Pal et al. 1980);
biodegradation rate $k \sim 2.6$ nmol L$^{-1}$ d$^{-1}$ with an initial concentration of 3.6 µmol L$^{-1}$ in water from Port Valdez estimated to be (data of August 1977, Reichardt et al. 1981);
biodegradation $t_{1/2} \sim 3–4$ d for 50% initial concentration of 1–100 µg L$^{-1}$ by river dieaway test (Bailey et al. 1983);
degradation rate $k = 1.6$ µg mL$^{-1}$ d$^{-1}$ at 30 µg mL$^{-1}$ under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

**Biotransformation:**
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 0.29$ d$^{-1}$, 0.13 d$^{-1}$, 0.11 d$^{-1}$, 0.11 d$^{-1}$ (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Half-Lives in the Environment:
Air: estimated atmospheric lifetime of ~ 4 d due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5$ cm$^{-3}$ (Atkinson & Aschmann 1985);
calculated tropospheric lifetime of 5–11 based on the calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 2 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);
tropospheric lifetime of 2.7–5.1 d based on both the experimentally determined and calculated rate constant for reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{1/2} = 45$ d under sunlight in water (Mansour & Feicht 1994);
$t_{1/2} = 15–19$ min, 8–10 min and 3–4 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively;
$t_{1/2} = 16–26$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$;
$t_{1/2} = 19–21$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota:

### TABLE 7.1.1.2.1
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
<th>P/Pa</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
<th>P/Pa</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>310</td>
<td>1.52</td>
<td>2.43</td>
<td>1.97</td>
<td>313</td>
<td>2.29</td>
<td>3.62</td>
<td>2.96</td>
</tr>
<tr>
<td>319</td>
<td>3.05</td>
<td>4.12</td>
<td>3.58</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Ferro et al. 1983*

(Continued)
TABLE 7.1.1.2.1 (Continued)
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and
the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>T/K</th>
<th>torsion effusion P/Pa</th>
<th>Knudsen P/Pa</th>
<th>average P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>323</td>
<td>3.81</td>
<td>6.23</td>
<td>5.02</td>
</tr>
<tr>
<td>327</td>
<td>8.33</td>
<td>8.53</td>
<td>6.93</td>
</tr>
<tr>
<td>332</td>
<td>8.38</td>
<td>12.9</td>
<td>10.6</td>
</tr>
<tr>
<td>336</td>
<td>11.4</td>
<td>18.0</td>
<td>14.7</td>
</tr>
<tr>
<td>341</td>
<td>14.5</td>
<td>22.5</td>
<td>15.4</td>
</tr>
<tr>
<td>346</td>
<td>19.8</td>
<td>30.0</td>
<td>24.9</td>
</tr>
<tr>
<td>350</td>
<td>28.2</td>
<td>43.2</td>
<td>35.7</td>
</tr>
</tbody>
</table>

cell C

<table>
<thead>
<tr>
<th>T/K</th>
<th>torsion effusion P/Pa</th>
<th>Knudsen P/Pa</th>
<th>average P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>332</td>
<td>13.6</td>
<td>19.1</td>
<td>16.3</td>
</tr>
<tr>
<td>336</td>
<td>15.8</td>
<td>22.3</td>
<td>19.0</td>
</tr>
<tr>
<td>341</td>
<td>23.4</td>
<td>29.0</td>
<td>26.2</td>
</tr>
<tr>
<td>346</td>
<td>27.5</td>
<td>35.6</td>
<td>31.5</td>
</tr>
<tr>
<td>350</td>
<td>33.7</td>
<td>46.2</td>
<td>40.0</td>
</tr>
<tr>
<td>354</td>
<td>47.3</td>
<td>63.6</td>
<td>55.4</td>
</tr>
<tr>
<td>359</td>
<td>63.2</td>
<td>84.9</td>
<td>74.0</td>
</tr>
</tbody>
</table>

eq. 1

<table>
<thead>
<tr>
<th>P/mmHg</th>
<th>P/mmHg</th>
<th>P/mmHg</th>
</tr>
</thead>
<tbody>
<tr>
<td>torsion</td>
<td>Knudsen</td>
<td>average</td>
</tr>
<tr>
<td>A</td>
<td>8.91</td>
<td>8.45</td>
</tr>
<tr>
<td>B</td>
<td>3771</td>
<td>3458</td>
</tr>
</tbody>
</table>

range, K 341–402 310–359

FIGURE 7.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorobiphenyl (PCB-2).
7.1.1.3 4-Chlorobiphenyl (PCB-3)

Common Name: 4-Chlorobiphenyl
Synonym: PCB-3, p-chlorobiphenyl, 4-chloro-1,1′-biphenyl
Chemical Name: 4-chlorobiphenyl
CAS Registry No: 2051-62-9
Molecular Formula: C_{12}H_9Cl
Molecular Weight: 188.652
Melting Point (°C):
78.8 (Lide 2003)
Boiling Point (°C):
292.9 (Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ∆H_v (kJ/mol):
65.94 (Geidarov et al. 1975)
Enthalpy of Sublimation, ∆H_{subl} (kJ/mol):
79.24 (Geidarov et al. 1975)
Enthalpy of Fusion, ∆H_{ fus} (kJ/mol):
13.32 (Geidarov et al. 1975; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ∆S_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{ fus} = 56 J/mol K), F: 0.297 (mp at 78.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0 (Webb 1970)
0.40 (Hoover, 1971)
0.90 (generator column-GC/ECD, Weil et al. 1974)
1.65 (Branson 1977)
0.0151 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
1.478* (generator column-GC/ECD, measured range 4–32°C, Stolzenburg & Andren 1983)
ln x = –3428/(T/K) – 4.2786, ∆H_{ss} = 28.5 kJ/mol (regression eq. given by Dickhut et al. 1986, based on exptl data of Stolzenburg & Andren 1983)
log x = –1486/(T/K) – 1.850; ∆H_{ss} = 28.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983); or
S/(mol/L) = 2.94 × 10^{-8} exp(0.041·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983)
1.20 (selected, Shiu & Mackay 1986)
1.30, 1.38 (generator column-HPLC/UV, Billington et al. 1988)
0.82, 0.88, 0.84, 0.95 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.207 (generator column-GC/ECD, Dunning & Elzerman 1988)
0.81 (shake flask-LSC, [14C] 4-monoCB, Eadie et al. 1990)
1.34 (shake flask-GC/ECD, Li et al. 1992; Li & Andren 1994)
1.32 (shake flask-GC/ECD, Li & Doucette 1993)
1.37 ± 0.042 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
ln x = –5.9137 – 2926.22/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
3.23, 3.81 (supercooled liquid: LDV literature-derived value, FAV final-adjusted value, Li et al. 2003)
\[
\log S_L/(\text{mol m}^{-3}) = -631/(T/K) + 0.35 \quad (\text{supercooled liquid, linear regression of literature data, Li et al. 2003})
\]
\[
\log S_L/(\text{mol m}^{-3}) = -963/(T/K) + 1.53 \quad (\text{supercooled liquid, FA V final adjusted eq., Li et al. 2003})
\]

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**

- 133.3* (96.4°C, summary of literature data, temp range 96.4–292.9°C, Stull 1947)
- 1.41 (supercooled liq. P_L, Weast 1972–1973)
- \[
\log (P/mm\text{Hg}) = (9.037 \pm 0.635) - (3445 \pm 18)/(T/K), \text{ temp range: 452–536 K} \quad \text{(static method-quartz manometer measurements, Geidarov et al. 1975)}
\]
- 0.61 (Neely 1981, 1983)
- 0.339*; 0.253 (P_S- Knudsen effusion; P_L-torsion effusion, extrapolated from exptl. derived from Antoine eq., Ferro et al. 1983)
- \[
\log (P_S/k\text{Pa}) = - (3849 \pm 200)/(T/K) + (9.44 \pm 0.63); \text{ temp range: 5.2–24.9°C} \quad \text{(gas saturation-GC, measured range 5.2–24.9°C, Burkhard et al. 1984; Burkhard et al. 1985a)}
\]
- \[
\log (P_L/k\text{Pa}) = - (3541 \pm 250)/(T/K) + (8.28 \pm 0.55); \text{ temp range 75–136°C} \quad \text{(torsion effusion data, liquid, Ferro et al. 1983)}
\]
- 1.41 (supercooled liquid P_L, converted from literature P_S, Bidleman 1984)
- 0.951, 0.567 (P_G by GC-RT correlation, different stationary phases, Bidleman 1984)
- 0.92, 0.942 (supercooled liquid P_L from P_G, GC-RT correlation, different GC columns, Bidleman 1984)
- 0.175* (gas saturation-GC, measured range 5.2–24.9°C, Delle Site 1997)
- \[
\log (P_S/k\text{Pa}) = - 4754.1/(T/K) + 15.188; \text{ temp range: 5.2–24.9°C} \quad \text{(gas saturation-GC, Clapeyron eq. Burkhard et al. 1984)}
\]
- \[
\log (P_L/k\text{Pa}) = - 3541/(T/K) + 11.71 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
\]
- 0.0677* (20°C, as saturation-GC/ECD, Wania et al. 1994)
- \[
\log (P_S/k\text{Pa}) = - 4493/(T/K) + 14.15; \text{ temp range: – 20 to 30°C} \quad \text{(gas saturation-GC, Wania et al. 1994)}
\]
- \[
\log (P_L/k\text{Pa}) = - 3488/(T/K) + 11.67 \quad \text{supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
\]
- \[
\log (P_S/k\text{Pa}) = - 4493/(T/K) + 14.15; \text{ temp range: – 20 to 30°C} \quad \text{(gas saturation-GC, Wania et al. 1994)}
\]

**Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):**

- 58.06 (batch stripping, Atlas et al. 1982; Dow Chemical, Neely 1982))
- 42.56 (calculated-P/C, Shiu & Mackay 1986)
- 34.14 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
- 24.39 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
- 23.30 (wetted-wall column-GC, Brunner et al. 1990)
- 5.84 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
- 18.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
- \[
\ln K_{AW} = - \Delta H_{R}/R + \Delta S_{R}/R; \quad R \text{ is the ideal gas constant, } \Delta H_{R} = 56 \pm 27 \text{ kJ/mol, } \Delta S_{R} = 0.15 \pm 0.10 \text{ kJ/mol-K} \quad \text{(Bamford et al. 2002)—see Comment by Goss et al. 2004}
\]
- 36.3, 23.44 (LDV literature-derived value, FA V final adjusted value, Li et al. 2003)
- \[
\log [H/(Pa \text{ m}^3/\text{mol})] = - 2664/(T/K) + 10.31 (\text{FAV final adjusted eq., Li et al. 2003})
\]

**Octanol/Water Partition Coefficient, log K_{OW}:**

- 4.90 (Branson 1977)
- 4.26 (Sugiura et al. 1978)
- 4.80 (Hansch & Leo 1979)
- 4.61 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)
Polychlorinated Biphenyls (PCBs)

4.69 (RP-TLC-\(k'\) correlation, Bruggeman et al. 1982)
4.34 (HPLC-RT correlation, Woodburn 1982)
4.49 (generator column-HPLC, Woodburn et al. 1984)
4.34 (HPLC-RT correlation, Woodburn et al. 1984)
4.40 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.49 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
4.55, 4.73, 4.64, 4.59 (RP-HPLC-\(k'\) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.53, 4.27 (RP-HPLC-\(k'\) correlation, different stationary phases, Sherbolm & Eganhouse 1988)
4.61 (recommended, Sangster 1989, 1993)
4.72 (HPLC-\(k'\) correlation, Noegrohati & Hammers 1992)
4.37 (generator column-HPLC, Li & Doucette 1993)
4.61 (recommended, Hansch et al. 1995)
4.49, 4.65 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log \(K_{OA}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

\[
\text{log } K_{OA} = -6.50 + 3962/(T/\text{K}); \text{ temp range } -10 \text{ to } 20^\circ \text{C}, \text{ (generator column-GC, Harner & Mackay 1995)}
\]

\[
\text{log } K_{OA} = -6.74 + 3660/(T/\text{K}); \text{ temp range } -10 \text{ to } 30^\circ \text{C}, \text{ (generator column-GC, Harner & Mackay 1995)}
\]

7.01* (generator column-GC; measured range –10 to 30°C, Harner & Mackay 1995)

7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

6.80; 6.93 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

6.82, 6.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

\[
\text{log } K_{OA} = 3520/(T/\text{K}) – 4.97 \text{ (FAV final adjusted eq., Li et al. 2003)}
\]

Bioconcentration Factor, log BCF:

2.08 (killifish, Goto et al. 1978)
2.68 (NAS 1979)
2.77 (estimated, fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.67 (calculated-solubility, Kenaga 1980)
3.88 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
2.77, 4.07 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log \(K_{OC}\):

3.52 (calculated, Kenaga 1980)
4.43 (suspended particulate matter, calculated-\(K_{OM}\), Burkhard 1984)
3.90 (soil, calculated-S, Chou & Griffin 1986)
4.71 (Great Lake suspended matter, phase partitioning-reversed phase chromatography by Sep Pak, Eadie et al. 1990)
4.70 (Green Bay suspended matter, reversed phase separation, Eadie et al. 1992)
3.49 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Sorption Partition Coefficient, log \(K_{OM}\):

4.02 (Great Lakes DOC, reversed phase separation, Eadie et al. 1990)
4.61 (Green Bay DOC, reversed phase separation, Eadie et al. 1992)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{\frac{1}{2}}\):

Volutilization:

Photolysis:

\[
k = 2.3 \times 10^{-4} \text{ d}^{-1} \text{ with } t_{\frac{1}{2}} = 8.2 \text{ yr in surface water at } 40^\circ \text{N in summer sunlight is } \text{(Dulin et al. 1986)}
\]

\[
t_{\frac{1}{2}} = 45 \text{ d in water } \text{(Mansour & Feicht 1994)}
\]

© 2006 by Taylor & Francis Group, LLC
k(calc) = 13.5 h^{-1}, maximum summer photolysis rate calculated under midday clear skies, experimental k(exptl) 
\sim 1.0 \times 10^{-8} \text{ mol s}^{-1}, \text{ irradiated with a low-pressure mercury lamp (Bunce et al. 1989)}

k = (0.036–0.045) \text{ min}^{-1} \text{ with } t_{1/2} = 15–19 \text{ min}, \ k = (0.048–0.082) \text{ min}^{-1} \text{ with } t_{1/2} = 8–14 \text{ min} \text{ and } k = (0.13–0.30) \text{ min}^{-1} \text{ with } t_{1/2} = 2–3 \text{ min} \text{ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 \mu g/mL TiO}_2, \text{ respectively; k = (0.027–0.046) min}^{-1} \text{ with } t_{1/2} = 15–26 \text{ min} \text{ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 \mu g/mL TiO}_2;

k = (0.022–0.038) \text{ min}^{-1} \text{ with } t_{1/2} = 18–31 \text{ min} \text{ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 \mu g/mL TiO}_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (3.9 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \pm 1 \text{ K}, \text{ with an estimated atmospheric lifetime of } 
\sim 6 \text{ d (relative rate method, Atkinson & Aschmann 1985)}

k_{OH} = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ to the C}_6\text{H}_4\text{Cl ring (ring B), k}_{OH} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ to ring A, and } k_{OH} = 3.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)}

k_{OH}(calc) = (2.8 – 5.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(exptl) = (3.1 – 4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)}

k_{OH} = 5.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K (Atkinson 1989)}

k_{OH}(calc) = (2.8 – 5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(exptl) = (3.2 – 4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)}

Hydrolysis:

Biodegradation: t_{1/2} = 175 \text{ h biodegradation by bacteria (Wong & Kaiser 1975; quoted, Pal et al. 1980)};

within 7 \text{ h by Alcaligenes sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980)}

k = 38 \text{ yr}^{-1} \text{ in the water column, and } k = 380 \text{ yr}^{-1} \text{ in the sediment, pseudo first-order rate constant for microbial degradation (Wong & Kaiser 1975; quoted, Neely 1981)}

k = 3.1 \text{ mmol L}^{-1} \text{ d}^{-1} \text{ with an initial concentration of 2.9 \mu mol/L, degradation rate in water from Port Valdez(data of Aug. 1977, Reichardt et al. 1981); t}_{1/2} = 2–5 \text{ d, time for 50% degradation of an initial concentration of 1–100 \mu g L}^{-1} \text{ by river dieaway test (Bailey et al. 1983)}

k = 2.0 \mu g \text{ mL}^{-1} \text{ d}^{-1} \text{ at 30 \mu g mL}^{-1}, \text{ under culture conditions include river water as supportive medium and mixed bacteria cultures obtained from river sediments (Kong & Sayler 1983)}

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.008 \text{ d}^{-1} \text{ with } t_{1/2} = 88 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)}

k_2 = 0.01 \text{ d}^{-1} \text{ with } t_{1/2} = 67 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)}

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of } \sim 6 \text{ d due to reaction with the OH radical for a 24-h average OH radical concn of } 5 \times 10^5 \text{ cm}^{-3} \text{ (Atkinson & Aschmann 1985)};

calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);

photolysis } t_{1/2} \sim 10–25 \text{ h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989)};

tropospheric lifetime of 3 \text{ d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991)};

tropospheric lifetime of 2.7–5.1 \text{ d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995)};

Surface water: } t_{1/2} = 4.9 \text{ d in Lake Michigan (Neely 1983)};

photolysis } t_{1/2} = 8.2 \text{ yr in summer sunlight at 40°L in surface waters (Dulin et al. 1986)};
photolysis $t_{1/2} = 45$ d, sunlight days in water (Mansour & Feicht 1994) $t_{1/2} = 15–19$ min, 8–14 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$ respectively; $t_{1/2} = 15–26$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; $t_{1/2} = 18–31$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater: Sediment: Soil: Biota: depuration $t_{1/2} = 88$ d for high-dose treatment, $t_{1/2} = 67$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

### TABLE 7.1.1.3.1
Reported aqueous solubilities and octanol-air partition coefficients of 4-chlorobiphenyl (PCB-3) at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stolzenburg &amp; Andren 1983</strong></td>
<td><strong>Shiu et al. 1997</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>generator column-GC/ECD</td>
</tr>
<tr>
<td>$t/°C S/g\cdot m^{-3}$</td>
<td>$t/°C S/g\cdot m^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>0.661</td>
</tr>
<tr>
<td>20</td>
<td>1.206</td>
</tr>
<tr>
<td>25</td>
<td>1.478</td>
</tr>
<tr>
<td>32</td>
<td>2.128</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta H_{sol}/(kJ \ mol^{-1}) = 28.5$ for 5–45°C</td>
<td>$\Delta H_{sol}/(kJ \ mol^{-1}) = 24.5$ for 5–45°C</td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/T$

- $A = -6.52$
- $B = 3962.2$

### FIGURE 7.1.1.3.1
Logarithm of mole fraction solubility and $K_{OA}$ versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).
TABLE 7.1.1.3.2
Reported vapor pressures of 4-chlorobiphenyl (PCB-3) at various temperatures and the coefficients for the vapor pressure equations:

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\]

1. Stull 1947  
Geidarov et al. 1975  
Ferro et al. 1983

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/mmHg</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>P/mmHg</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>P/mmHg</th>
</tr>
</thead>
<tbody>
<tr>
<td>96.4</td>
<td>133.3</td>
<td>data presented in graph and</td>
<td>33</td>
<td>0.762</td>
<td>0.697</td>
<td>0.729</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>129.8</td>
<td>666.7</td>
<td>eq 1</td>
<td>37</td>
<td>1.52</td>
<td>0.902</td>
<td>1.21</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>146.0</td>
<td>1333</td>
<td>A</td>
<td>50</td>
<td>3.05</td>
<td>3.57</td>
<td>3.31</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>164.0</td>
<td>2666</td>
<td>B</td>
<td>54</td>
<td>3.81</td>
<td>4.90</td>
<td>4.38</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>183.8</td>
<td>5333</td>
<td>cell B</td>
<td>59</td>
<td>6.10</td>
<td>7.41</td>
<td>6.75</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>196.0</td>
<td>7999</td>
<td>range: 179–263°C</td>
<td>63</td>
<td>9.14</td>
<td>10.4</td>
<td>9.77</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>212.6</td>
<td>13333</td>
<td></td>
<td>73</td>
<td>21.3</td>
<td>18.3</td>
<td>19.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>237.8</td>
<td>26664</td>
<td></td>
<td></td>
<td>74.75</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>284.5</td>
<td>53329</td>
<td></td>
<td>35</td>
<td>0.762</td>
<td>0.917</td>
<td>0.840</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>292.9</td>
<td>101325</td>
<td></td>
<td>41</td>
<td>1.62</td>
<td>1.41</td>
<td>1.47</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>75.5</td>
<td></td>
<td>44</td>
<td>2.29</td>
<td>1.72</td>
<td>2.00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>3.05</td>
<td>2.85</td>
<td>2.95</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>52</td>
<td>3.81</td>
<td>4.44</td>
<td>4.12</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>57</td>
<td>5.33</td>
<td>6.04</td>
<td>5.69</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>61</td>
<td>7.62</td>
<td>8.43</td>
<td>8.03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>62</td>
<td>8.38</td>
<td>10.9</td>
<td>9.66</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>65</td>
<td>10.7</td>
<td>10.8</td>
<td>10.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>67</td>
<td>12.9</td>
<td>11.9</td>
<td>12.4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>68</td>
<td>13.7</td>
<td>12.9</td>
<td>13.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>69</td>
<td>15.2</td>
<td>13.9</td>
<td>14.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>73</td>
<td>21.1</td>
<td>18.6</td>
<td>15.3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[\Delta H_v/(kJ \text{ mol}^{-1}) = 65.94\]
\[\Delta H_{fus}/(kJ \text{ mol}^{-1}) = 13.32\]
\[\Delta S_{fus}/(J \text{ mol}^{-1} \text{ K}^{-1}) = 38.3\]
\[\Delta H_{subl}/(kJ \text{ mol}^{-1}) = 79.24\]

© 2006 by Taylor & Francis Group, LLC
### TABLE 7.1.1.3.2 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.2</td>
<td>0.0111</td>
<td>-20</td>
<td>2.446 × 10^{-4}</td>
</tr>
<tr>
<td>15.0</td>
<td>0.0493</td>
<td>-10</td>
<td>1.297 × 10^{-3}</td>
</tr>
<tr>
<td>24.9</td>
<td>0.172</td>
<td>0</td>
<td>4.889 × 10^{-3}</td>
</tr>
<tr>
<td>25.0</td>
<td>0.175</td>
<td>10</td>
<td>1.883 × 10^{-2}</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>6.771 × 10^{-2}</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>0.2233</td>
</tr>
</tbody>
</table>

**Burkhard et al. 1984**

- gas saturation-GC
- range: 4.2–25°C

**Wania et al. 1994**

- gas saturation-GC

**eq. 1 P/Pa**

A 15.188
B 4754.1

**range: 4.2–25°C**

\[ \Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.0 \]

**FIGURE 7.1.1.3.2** Logarithm of vapor pressure versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).
7.1.1.4 2,2′-Dichlorobiphenyl (PCB-4)

![Chemical structure of 2,2′-Dichlorobiphenyl]

**Common Name:** 2,2′-Dichlorobiphenyl

**Synonym:** PCB-4, 2,2-dichloro-1,1′-biphenyl

**Chemical Name:** 2,2′-dichlorobiphenyl

**CAS Registry No:** 13029-08-8

**Molecular Formula:** C_{12}H_8Cl_2

**Molecular Weight:** 223.098

**Melting Point (°C):** 60.5 (Hutzinger et al. 1974)

**Boiling Point (°C):** 312 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

**Density (g/cm³ at 20°C):** 1.0536

**Molar Volume (cm³/mol):**
- 226.4 (calculated-Le Bas method at normal boiling point)
- 185.8 (Ruelle & Kesselring 1997)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.448 (mp at 60.5°C)
- 0.442 (Mackay et al. 1980; Shiu & Mackay 1986)

**Water Solubility (g/m³ or mg/L at 25°C):**
- 1.0 (Webb 1970)
- 0.90 (Hoover 1971)
- 1.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.79 (generator column-GC/ECD, Weil et al. 1974)
- 0.0212 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
- 1.86 (20°C, supercooled liquid, shake flask-GC/ECD, Chiu et al. 1982,1983; Chiu 1985)
- 1.124 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.511, 0.322, 0.362, 0.511 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

**VaporPressure (Pa at 25°C and reported temperature dependence equations):**
- 0.133 (Knudsen-effusion technique, extrapolated from 37–54.92°C, Smith et al. 1964)
- 0.36 (quoted, Neely 1981)
- 0.82 (P_L calculated from P_S using F, Neely 1981)
- 0.189 (GC-RI correlation, Burkhard et al. 1985a)
- 0.424 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985a)
- 0.326, 0.335 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.134 (extrapolated-Antoine eq., solid, Stephenson & Malanowski 1987)

\[
\log (P_L/kPa) = -5019/(T/K) + 12.962; \text{ temp range 37–55°C (Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
0.152 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
\]

\[
0.275, 0.363 (supercooled liquid P_L; GC-RI correlation, different stationary phases, Fischer et al. 1992)
\]

\[
\log (P_L/\text{Pa}) = -3462/T + 11.73 \text{ (supercooled liquid P_L; GC-RT, Falconer & Bidleman 1994)}
\]

\[
0.0603–0.315; 0.280–0.424 \text{ (quoted literature P_S range; literature P_L range, Delle Site 1997)}
\]

**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):**
- 30.2 (20°C, calculated-P/C, Murphy et al. 1987)
- 34.14 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
- 23.3 (wetted-wall column-GC, Brunner et al. 1990)
Polychlorinated Biphenyls (PCBs)

8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
23.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\[ \ln K_{AW} = -\frac{\Delta H_H}{RT} + \frac{\Delta S_H}{R} \]
R is the ideal gas constant, \( \Delta H_H = 50 \pm 25 \text{ kJ/mol} \), \( \Delta S_H = 0.13 \pm 0.09 \text{ kJ/mol-K} \)
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 4.04 (HPLC-RT correlation, Sugiura et al. 1978)
- 5.70 (HPLC-RT correlation, Sugiura et al. 1979)
- 5.51 (Hansch & Leo 1979)
- 4.00 (HPLC-k' correlation, McDuffie 1981)
- 5.00 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)
- 3.02 (RP-TLC-retention correlation, Bruggeman et al. 1982)
- 3.55 (HPLC-RT correlation, Woodburn 1982)
- 4.80 (shake flask-GC/ECD, Chiu et al. 1983; Chiu 1985; Chiu & Block 1986)
- 4.90; 3.55 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
- 3.63; 4.89 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
- 4.90 (generator column-GC/ECD, Doucette & Andre 1987, 1988)
- 4.25, 4.89 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 4.965 ± 0.013 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 5.09 (HPLC-k' correlation, Noegrohati & Hammers 1992)
- 4.73 (recommended, Sangster 1993)
- 4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{oa} \) or as indicated and reported temperature dependence equations:

- 7.18; 6.56 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- \( \log K_{oa} = -4.84 + 3590/(T/K) \) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 7.66, 6.86 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
- 6.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 2.04 (killifish, Goto et al. 1978)
- 3.72, 2.95, 3.60, 3.26 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
- – 1.40, – 1.30, – 1.35 (adipose tissue of male, female Albino rats, rodents, Geyer et al. 1980)
- 2.05, 2.45 (fish: flowing water, microcosm condition Garten & Trabalka 1983)
- 3.43, 2.90 (algae, calculated, Geyer et al. 1984)
- 3.43, 3.38, 3.80 (algae, fish, activated sludge, Freitag et al. 1984, 1985)
- 3.85 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
- 3.38; 3.413, 3.715 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, \( K_{OW} \), Lu et al. 1999)

Sorption Partition Coefficient, log \( K_{OC} \) at 25°C or as indicated:

- 3.68 (Woodburn silt loam soil, soil organic matter, sorption isotherm-GC, Chiou et al. 1983)
- 4.76 (suspended particulate matter, calculated-\( K_{OW} \), Burkhard 1984)
- 3.84 (soil, calculated-S, Chou & Griffin 1986)
- 3.92 (soil, calculated-MCI, Sabljic et al. 1995)
- 3.96; 3.92 (soil, calculated-Characterestic Root Index CRI; quoted lit., Saçan & Balcioğlu 1996)
- 4.30 (soil, calculated-\( K_{OW} \), Girvin & Scott 1997)
- 4.90; 3.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, log \( K_{OM} \) at 25°C or as indicated:

- 3.68 (20°C, Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
- 3.68, 4.18 (quoted, calculated-MCI \( \chi \), Sabljic 1984)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volutilization: estimated t½ ~ 3.1 h of evaporation with an initial concentration of 0.1 ppm from 4.5 cm depth of water solution in a glass dish at 24°C is 3.1 h and t½ = 0.4 h with stirring of the solution; the experimental t½ = 3.9 h and 0.9 h of evaporation under same condition with stirring of the solution (Chiu et al. 1979).

Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:

\[ k_{OH}(calc) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR, Atkinson 1987)} \]

kOH(calc) = (1.4 – 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, and the tropospheric lifetime \( \tau(\text{calc}) = 8–17 \text{ d} \)
for dichlorobiphenyls due to gas-phase loss process at room temp. (Atkinson 1987)

\[ k_{OH} = (2.0 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]
\[ k_{O3} < 2.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 297 \pm 2 \text{ K} \]
(relative rate method, Kwok et al. 1995)

tropospheric lifetime \( \tau(\text{calc}) = 3.4–7.2 \text{ d} \), based on the experimentally determined gas-phase reaction

\[ k_{OH}(\text{exptl}) = (2.0 – 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]
and the calculated \( k_{OH}(\text{calc}) = (1.4 – 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Kwok et al. 1995)} \)

Hydrolysis:

Biodegradation: Biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980); microbial degradation with pseudo first-order \( k = 0.65 \text{ yr}^{-1} \) in the water column and \( k = 6.5 \text{ yr}^{-1} \) in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

\[ k_2 = 0.027 \text{ d}^{-1} (10°C, \text{sandworm, Goerke & Erst 1977; quoted, Waid 1986}) \]
\[ k_1 = 0.29 \text{ d}^{-1}, 0.13 \text{ d}^{-1}, 0.11 \text{ d}^{-1}, 0.11 \text{ d}^{-1} (\text{golden orfe, carp, brown trout, guppy, Sugiura et al. 1979}) \]
\[ k_2 = 0.017 \text{ d}^{-1} (\text{rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990}) \]
\[ k_2 = 122 \text{ d}^{-1}, k_2 = 0.014 \text{ d}^{-1} (\text{rainbow trout, calculated, Gobas & Mackay 1987}) \]
\[ k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 183 \text{ d} (8°C, \text{juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004}) \]
\[ k_2 = 0.004 \text{ d}^{-1} (8°C, \text{juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004}) \]

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: \( t_{1/2} = 34.5 \text{ d} \) in Lake Michigan (Neely 1983)

Groundwater:

Sediment:

Soil:

Biota: \( t_{1/2} = 40 \text{ d} \) in rainbow trout, and \( t_{1/2} = 20 \text{ d} \) in its muscle (Niimi & Oliver 1983).

Depuration \( t_{1/2} = 183 \text{ d} \) for high-dose treatment, \( t_{1/2} = 93 \text{ d} \) for high-dose + enzyme treatment (juvenile rainbow trout, Buckman et al. 2004)
### 2,3-Dichlorobiphenyl (PCB-5)

- **Common Name:** 2,3-Dichlorobiphenyl
- **Synonym:** PCB-5, 2,3-dichloro-1,1′-biphenyl
- **Chemical Name:** 2,3-dichlorobiphenyl
- **CAS Registry No:** 16605-91-7
- **Molecular Formula:** C\(_{12}\)H\(_8\)Cl\(_2\)
- **Molecular Weight:** 223.098
- **Melting Point (°C):** 28.0
  - 27.8–28.2 (Erickson 1985)
- **Boiling Point (°C):** 172 (at 4000 Pa, Erickson 1986)
- **Density (g/cm\(^3\)):**
  - 226.4 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):**
- **Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):**
- **Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), F: 0.934 (mp at 28°C)
- **Water Solubility (g/m\(^3\) or mg/L at 25°C):**
  - 1.70 (supercooled liquid \(S_L\), calculated-TSA, Burkhard et al. 1985b)
  - 1.31, 1.23, 0.756, 0.829 (quoted lit.; RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
  - 1.00, 0.658 (quoted average of Brodsky & Ballschmiter 1988, calculated-MCI \(\chi\), Patil 1991)
  - 1.36 (calculated-QSPR, Dunnivant et al. 1992)
- **Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
  - 0.147, 0.144, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI \(\chi\), Burkhard et al. 1985a)
  - 0.151 (supercooled liquid \(P_L\), GC-RT correlation, Burkhard et al. 1985b)
  - 0.162 (supercooled liquid \(P_L\), GC-RI correlation, Fischer et al. 1992)
- **Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):**
  - 19.56 (calculated-P/C, Burkhard et al. 1985b)
  - 28.57 (calculated-MCI \(\chi\), Sabljic & Güsten 1989)
  - 23.30 (wetted-wall column-GC, Brunner et al. 1990)
  - 24.19 (calculated-QSPR, Dunnivant et al. 1992)
  - 8.97 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  - 24.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
- **Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):**
  - 5.20 (RP-TLC-RT correlation, Bruggeman et al. 1982)
  - 4.82, 4.92, 5.17, 5.05 (RP-PLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  - 4.99 (recommended, Sangster 1993)

**Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\) at 25°C or as indicated and reported temperature dependence equations:**

  - 7.40; 6.98 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
  - \(\log K_{\text{OA}} = -5.41 + 3820/(T/K)\); temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

---

© 2006 by Taylor & Francis Group, LLC
Bioconcentration Factor, log BCF at 25°C or as indicated:

3.08 (oyster, Vreeland 1974)
3.45–4.11 mean 4.11 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.41; 4.11 (rainbow trout, 15°C, kinetic BCF k1/k2, steady-state BCF C/F/CW, Oliver & Niimi 1985)
4.11, 5.25; 3.888, 3.895 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, KOW, Lu et al. 1999)
3.08, 5.33 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.20 (rainbow trout: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log KOC:
4.76 (suspended particulate matter, Burkhard 1984)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization:
Photolysis: rate constant k = (0.031–0.036) min⁻¹ with t½ = 19–23 min, k = (0.054–0.067) min⁻¹ with t½ = 10–13 min and k = (0.22–0.25) min⁻¹ with t½ = 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO₂, respectively; k = (0.022–0.028) min⁻¹ with t½ = 25–32 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO₂; k = (0.022–0.024) min⁻¹ with t½ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO₂ (Huang et al. 1996).

Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:
kOH(calc) = 1.8 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d, based on kOH(calc) = (1.4 – 2.9) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ for dichlorobiphenyls at room temp. (Atkinson 1987)
kOH(aq) = 7.9 × 10¹⁰ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction kOH(exptl) = (2.0 – 4.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹, and the calculated kOH(calc) = (1.4 – 3.1) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
k₁ = 0.011 d⁻¹ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k₁ = 300 d⁻¹; k₂ = 0.011 d⁻¹ (rainbow trout, Oliver & Niimi 1985)
log 1/k₂ = 2.0, 2.2 h (fish, quoted, calculated-KOW, Hawker & Connell 1988b)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water: τw = ~ 4–11 d in freshwater systems, τw = 0.1–10 d in cloud water, τw > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);
Polychlorinated Biphenyls (PCBs)

- $t_{1/2} = 19$–$23$ min, $10$–$13$ min and $3$ min in aqueous Aroclor 1248 solution containing $45$ ng/mL of total PCB irradiated by UVA-340 in the presence of $25$, $50$ and $100$ µg/mL TiO$_2$, respectively;
- $t_{1/2} = 16$–$26$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing $450$ ng/mL of total PCB irradiated by sunlight in the presence of $100$ µg/mL TiO$_2$;
- $t_{1/2} = 29$–$31$ min in St. Lawrence River water containing $3$ ng/mL of total PCB irradiated by sunlight in the presence of $100$ µg/mL TiO$_2$ (Huang et al. 1996).

**Groundwater:**
**Sediment:**
**Soil:**
**Biota:** $t_{1/2} = 61$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2} = 26$ d in its muscle (Niimi & Oliver 1983).
7.1.1.6 2,3′-Dichlorobiphenyl (PCB-6)

Common Name: 2,3′-Dichlorobiphenyl
Synonym: PCB-6
Chemical Name: 2,3′-dichlorobiphenyl
CAS Registry No: 25569-80-6
Molecular Formula: C_{12}H_{8}Cl_{2}
Molecular Weight: 223.098

Melting Point (°C): 36 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.605 (supercooled liquid S_{L}, Burkhard et al. 1985a)
0.580 (20°C, supercooled liquid S_{L}, Murphy et al. 1987)
1.226 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.928 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.165 (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.157, 0.169, 0.0754 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.173, 1.208 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0799 (20°C, supercooled liquid, Murphy et al. 1987)
0.141, 0.178 (supercooled liquid P_{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = – 3769/(T/K) + 11.88 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
27.76 (calculated-P/C, Burkhard et al. 1985a)
30.0 (20°C, calculated-P/C, Murphy et al. 1987)
39.42 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
25.33 (wetted-wall column-GC, Brunner et al. 1990)
33.09 (calculated-QSPR, Dunnivant et al. 1992)
4.016, 11.74 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
24.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = - ∆H_{f}/R + ∆S_{f}/R; R is the ideal gas constant, ∆H_{f} = 47 ± 24 kJ/mol, ∆S_{f} = 0.12 ± 0.08 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (calculated-TSA, Burkhard 1984)
5.02 (quoted and selected, Brownwell & Farrington 1985)
4.84 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
Polychlorinated Biphenyls (PCBs)

5.06 (calculated-TSA, Hawker & Connell 1988a)
5.02 (recommended, Hansch et al. 1995)
5.044 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K\text{OA} at 25°C or as indicated:
8.51; 7.55 (0; 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
7.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K\text{BCF}:

Sorption Partition Coefficient, log K\text{OC}:
4.83 (suspended particulate matter, calculated-K\text{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, t\text{½}:

Volatilization:
Photolysis: k = (0.018–0.052) min\textsuperscript{–1} with t\textsubscript{½} = 13–38 min, irradiated by sunlight in the presence of 100 µg/mL TiO\textsubscript{2} of diCBs in St. Lawrence River water containing 3 ng/mL of total PCB (Huang et al. 1996)
Oxidation: rate constant k, for gas-phase second order rate constants, k\text{OH} for reaction with OH radical, k\text{NO3} with NO\textsubscript{3} radical and k\text{O3} with O\textsubscript{3} or as indicated, *data at other temperatures see reference:
k\text{OH}(\text{calc}) = 2.1 \times 10\textsuperscript{–12} cm\textsuperscript{3} molecule\textsuperscript{–1} s\textsuperscript{–1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d, based on k\text{OH}(\text{calc}) = (1.4 – 2.9) \times 10\textsuperscript{–12} cm\textsuperscript{3} molecule\textsuperscript{–1} s\textsuperscript{–1} for dichlorobiphenyl at room temp. (Atkinson 1987)
k\text{OH}(\text{aq}) = 8.0 \times 10\textsuperscript{9} dm\textsuperscript{3} mol\textsuperscript{–1} s\textsuperscript{–1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from t\textsubscript{½} = 4–11 d in freshwater systems, t\textsubscript{½} = 0.1–10d in cloud water, t\textsubscript{½} > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k\text{OH(exptl)} = (2.0 – 4.2) \times 10\textsuperscript{–12} cm\textsuperscript{3} molecule\textsuperscript{–1} s\textsuperscript{–1}, and the calculated k\text{OH}(calc) = (1.4 – 3.1) \times 10\textsuperscript{–12} cm\textsuperscript{3} molecule\textsuperscript{–1} s\textsuperscript{–1} at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k\textsubscript{1} and k\textsubscript{2}):
k\textsubscript{1} = 0.012 d\textsuperscript{–1} with t\textsubscript{½} = 56 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k\textsubscript{2} = 0.013 d\textsuperscript{–1} with t\textsubscript{½} = 53 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water: half-lives range from t\textsubscript{½} = 4–11 d in freshwater systems, t\textsubscript{½} = 0.1–10 d in cloud water, t\textsubscript{½} > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);
t\textsubscript{½} = 13–38 min for dichlorobiphenyl in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO\textsubscript{2} (Huang et al. 1996)

Ground water:
Sediment:
Soil:
Biota: depuration t\textsubscript{½} = 56 d for high-dose treatment, t\textsubscript{½} = 53 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.7  2,4-Dichlorobiphenyl (PCB-7)

Common Name: 2,4-Dichlorobiphenyl  
Synonym: PCB-7, 2,4-dichloro-1,1′-biphenyl  
Chemical Name: 2,4-dichlorobiphenyl  
CAS Registry No: 33284-50-3  
Molecular Formula: C₁₂H₈Cl₂  
Molecular Weight: 223.098  
Melting Point (°C):  
  24.1–24.4 (Dickerman & Weiss 1957; Weingarten 1961; Hutzinger et al. 1974)  
Boiling Point (°C):  
  Density (g/cm³ at 20°C): 1.0536  
  Molar Volume (cm³/mol):  
    226.4 (calculated-Le Bas method at normal boiling point)  
    185.8 (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ΔHₜₐₜ (kJ/mol):  
Entropy of Fusion, ΔSₜₐₜ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₜₐₜ = 56 J/mol K), F:  
  1.0 (calculated, Shiu & Mackay 1986)  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
  0.637 (shake flask-GC/ECD, Haque & Schmedding 1975)  
  1.13 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)  
  0.587, 0.535, 0.689, 0.659 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)  
  1.148 (generator column-GC/ECD, Dunnivant & Elzerman 1988)  
Vapor Pressure (Pa at 25°C):  
  0.184, 0.321 (supercooled liquid Pₜ, GC-RT correlation, different GC columns, Bidleman 1984)  
  0.175 (supercooled liquid Pₜ, Burkhard et al. 1984)  
  0.179 (GC-RI correlation, Burkhard et al. 1985a)  
  0.175 (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al. 1985b)  
  0.210, 0.216 (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
  0.170, 0.195 (supercooled liquid Pₜ, GC-RI correlation, different stationary phases, Fischer et al. 1992)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
  96.66 (gas stripping-GC, Atlas et al. 1982)  
  35.26 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)  
  28.37 (wetted-wall column-GC/ECD, Brunner et al. 1990)  
  24.78 (wetted-wall column-GC, Fendinger & Glotfelty 1990)  
  11.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
  28.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
ln Kₐₚₚ = – ΔHₜ/RT + ΔSₜ/R; R is the ideal gas constant, ΔHₜ = 43 ± 22 kJ/mol, ΔSₜ = 0.11 ± 0.08 kJ/mol·K  
  (Bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log Kₐₚₚ:  
  5.15 (RP-TLC-RT correlation, Bruggeman et al. 1982)  
  4.67 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
Polychlorinated Biphenyls (PCBs)

5.09, 5.21, 5.20, 5.10 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.13 (HPLC-k correlation, Noegrohati & Hammers 1992)

5.16 (recommended, Sangster 1993)

5.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

8.37, 7.39; 7.25 (0°C, multi-column GC-k correlation; calculated at 20°C, Zhang et al. 1999)

6.98 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

4.83 (suspended particulate matter, calculated-K $O_W$, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half Lives, $t_{1/2}$:

Volatileization:

Photolysis: calculated sunlight $k < 2 \times 10^{-8}$ s$^{-1}$ and $5.7 \times 10^{-11}$ s$^{-1}$, with $t_{1/2} > 400$ d at 40°N latitude in winter (Dulin et al. 1986);

$k = (0.30–0.036)$ min$^{-1}$ with $t_{1/2} = 19–23$ min, $k = (0.054–0.067)$ min$^{-1}$ with $t_{1/2} = 10–13$ min and

$k = (0.13–0.21)$ min$^{-1}$ with $t_{1/2} = 3–5$ min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; rate constants $k = (0.015–0.043)$ min$^{-1}$ with $t_{1/2} = 36–29$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; rate constants $k = (0.018–0.022)$ min$^{-1}$ with $t_{1/2} = 31–38$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{O_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{O_3}$(calc) = 1.8 × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR, Atkinson 1987)

Tropospheric lifetime $\tau$(calc) = 8–17 d for dichlorobiphenyls, based on $k_{O_3}$(calc) = (1.4 – 2.9) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

$k_{O_3}$(aq) = 7.1 × 10$^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

Tropospheric lifetime $\tau$(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{O_3}$(exptl) = (2.0 – 4.2) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and the $k_{O_3}$(calc) = (1.4 – 3.1) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by Alcaligenes sp. strain Y-42 from lake sediments but small amount residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 192$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 149$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991); $t_{1/2}$ = 19–23 min, 10–13 min and 3–5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$ respectively; $t_{1/2}$ = 36–29 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; $t_{1/2}$ = 31–38 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 192 d for high-dose treatment, $t_{1/2}$ = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.8 2,4′-Dichlorobiphenyl (PCB-8)

![Chemical structure of 2,4′-Dichlorobiphenyl](image)

- **Common Name:** 2,4′-Dichlorobiphenyl
- **Synonym:** PCB-8, 2,4′-dichloro-1,1′-biphenyl
- **Chemical Name:** 2,4′-dichlorobiphenyl
- **CAS Registry No:** 34883-43-7
- **Molecular Formula:** C₁₂H₈Cl₂
- **Molecular Weight:** 223.098

**Melting Point (°C):**
46 (Hutzinger et al. 1974)

**Boiling Point (°C):**

**Density (g/cm³ at 20°C):** 1.0536

**Molar Volume (cm³/mol):**
- 226.4 (calculated-Le Bas method at normal boiling point)
- 185.8 (Ruelle & Kesselring 1997)

**Enthalpy of Fusion, ∆H_{fus} (kJ/mol):**

**Entropy of Fusion, ∆S_{fus} (J/mol K):**

**Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:**
0.66 (Mackay et al. 1980; Shiu & Mackay 1986)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):**
- 0.50 (Webb 1970; Hoover 1971)
- 1.88 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.637 (shake flask-GC, Haque & Schmedding 1975)
- 0.620 (generator column-GC/ECD, Weil et al. 1974)
- 0.139 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)
- 1.17 (20°C, supercooled liquid P₁, shake flask-GC/ECD, Chiou et al. 1983; Chiu 1985)
- 0.974, 0.848, 0.643, 0.658 (RP-HPLC-k⁺ correlation, different stationary and mobile phases, Brodsky & Ballschmider 1988)
- 1.58, 1.45 (supercooled liquid S₁: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

log S₁/(mol m⁻³) = –1000/(T/K) + 1.17 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**
- 0.0998 (GC-RI correlation, Burkhard et al. 1985a)
- 0.147 (supercooled liquid P₁, GC-RI correlation, Burkhard et al. 1985b)
- 0.157, 0.143 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

log (P/mmHg) = 9.74 – 3840/(T/K) (GC-RT correlation, Tateya et al. 1988)

log (P₁/Pa) = –3769/(T/K) + 11.84 (GC-RT correlation, Falconer & Bidleman 1994)

log (P₁/Pa) = –3728/(T/K) + 11.68 (supercooled liquid, final adjusted eq., Li et al. 2003)

**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):**
- 96.7 (gas stripping-GC, Atlas et al. 1982)
- 23.30 (wetted wall column-GC/ECD, Brunner et al. 1990)
- 35.67 ± 2.7 (gas stripping-GC/ECD; Girvin et al. 1997)

ln K_{AW} = 13.2307 ± 5304.31/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

K_{AW} = exp[-(44.1/kJ·mol⁻¹·K⁻¹)/R] + (0.110/kJ·mol⁻¹·K⁻¹)/R]; where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
25.7 (exptl. data, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; \ R \ \text{is the ideal gas constant}, \ \Delta H_{f} = 44 \pm 3 \ \text{kJ/mol}, \ \Delta S_{f} = 0.11 \pm 0.01 \ \text{kJ/mol-K} \]

(Bamford et al. 2002)—see Comment by Goss et al. 2004

26.3, 22.9 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

\[ \log H/(Pa \ m^3/mol) = -2428/(T/K) + 9.56 \] (LDV linear regression of literature data, Li et al. 2003)

\[ \log H/(Pa \ m^3/mol) = -2728/(T/K) + 10.51 \] (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, \( \log K_{ow} \): 

5.51 (Hansch & Leo 1979)

4.48 (HPLC-RT correlation, Woodburn 1982)

5.10 (shake flask-GC, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)

5.10 ± 0.4 (selected, Shiu & Mackay 1986)

5.14 (generator column-GC/ECD, Woodburn et al. 1984)

4.47; 5.10 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)

5.14 (generator column-GC/ECD, Doucette & Andren 1987, 1988)

4.93, 5.05, 5.24, 5.15 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)

5.27 (average value, generator column-GC, Larsen et al. 1992)

5.09 (recommended, Sangster 1993)

5.10 (recommended, Hansch et al. 1995)

5.09, 5.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, \( \log K_{oa} \) or as indicated and reported temperature dependence equations:

7.40 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)

\[ \log K_{oa} = -5.41 + 3820/(T/K) \] (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)

8.58, 7.61 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)

7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

\[ \log K_{oa} = 3785/(T/K) - 5.35 \] (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, \( \log BCF \):


2.60–4.08 (various marine species, mean dry wt. BCF, Hope et al. 1998)

4.12–5.33 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

3.83, 4.53 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)

3.57, 5.76 (Daphnia: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, \( \log K_{oc} \):

3.90 (soil/sediment, sorption isotherm, Haque & Schmedding 1976)

4.16 (Woodburn silt loam soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

4.83 (suspended particulate matter, calculated-K_{ow}, Burkhard 1984)

5.90 (Lake Michigan water column, Swackhamer & Armstrong 1987)

5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

3.99; 4.13 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioglu 1996)

4.54–4.56 (Catlin silt loam, \( f_{OC} = 0.0226 \), depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.65–4.70 (Cloundland loam, \( f_{OC} = 0.0024 \), depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.61 (Kenoma silt loam, \( f_{OC} = 0.0153 \), depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.38–4.39 (Kenoma silt loam, \( f_{OC} = 0.0092 \), depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.57–4.73 (Kenoma silt loam, \( f_{OC} = 0.002 \), depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.52–4.54 (Norborne silt loam, \( f_{OC} = 0.0137 \), depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.54–4.57 (Norborne silt loam, \( f_{OC} = 0.009 \), depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.53–4.66 (Norborne silt loam, \( f_{OC} = 0.0057 \), depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
Polychlorinated Biphenyls (PCBs)

4.23–4.53; 3.90–5.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.23; 3.93, 4.53, 4.46 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log $K_{OM}$:
3.89 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatileization: depletion rate constant $k = 45$ d$^{-1}$ from aqueous solution in a 26-cm or 67-cm purge vessel, (Girvin et al. 1997).

Photolysis: photolysis rate $k_p$ (expt) $< 2 \times 10^{-8}$ d$^{-1}$ with $t_{1/2}$ > 400 d; $k_p$ (calc) $< 2 \times 10^{-8}$ d$^{-1}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Hydrolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}$ (calc) = $1.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau$ (calc) = 8–17 d for dichlorobiphenyls, based on $k_{OH}$ (calc) = $(1.4 - 2.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime $\tau$ (calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}$ (expt) = $(2.0 - 4.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and the $k_{OH}$ (calc) = $(1.4 - 3.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Sorption-Desorption Rate Constants:

$k_1 = 0.006$ d$^{-1}$ with $t_{1/2} = 109$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007$ d$^{-1}$ with $t_{1/2} = 104$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{1/2}$ > 400 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 109$ d for high-dose treatment, $t_{1/2} = 104$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.9 2,5-Dichlorobiphenyl (PCB-9)

![Chemical Structure](image)

Common Name: 2,5-Dichlorobiphenyl
Synonym: PCB-9, 2,5-dichloro-1,1′-biphenyl
Chemical Name: 2,5-dichlorobiphenyl
CAS Registry No: 34883-39-1
Molecular Formula: C_{12}H_8Cl_2
Molecular Weight: 223.098
Melting Point (°C):
22–23 (Weingarten 1962)
Boiling Point (°C):
171 (15mm Hg, Erickson 1986)
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C, $F$:
1.0 (calculated, assuming $\Delta S_{\text{fus}} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
- 0.58 (generator column-GC/ECD, Weil et al. 1974)
- 2.028 (shake flask-GC, Chiou et al. 1977)
- 0.190 (generator column-GC/ECD, Bruggeman et al. 1981)
- 1.940 (generator column-GC/ECD, Miller et al. 1984; 1985)
- 0.0739, 0.0739, 0.0722, 0.07055 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 1.115 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.0775 (Augood et al. 1953)
- 0.184 (supercooled liquid $P_L$, Yalkowsky et al. 1983)
- 0.184 (supercooled liquid $P_L$, GC-RT correlation, Bidleman 1984)
- 0.202 (GC-RI correlation, Burkhard et al. 1985a)
- 0.198 (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
- 0.231, 0.232 (supercooled liquid $P_L$, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)
- 0.180 (selected, Shiu & Mackay 1986)
- 0.204 (supercooled liquid $P_L$: GC-RI correlation, Fischer et al. 1992)
- $\log (P_L/P_a) = –3862/(T/K) + 12.22$, (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)
- 0.105–0.232 (quoted lit. $P_L$ range, Delle Site 1997)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
- 28.37 (wetted wall column-GC/ECD, Brunner et al. 1990)
- 16.1, 29.6, 58.2, 82.2, 123, 165.4 (10.4, 20, 30.1, 34.9, 42.1, 47.9°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
- 30.95 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
- $\log K_{A,W} = 6.055 – 2331/(T/K)$, (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Polychlorinated Biphenyls (PCBs) 1523

29.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$$\ln K_{AW} = -\Delta H_f^{\prime}/RT + \Delta S_f^{\prime}/R; \ R \text{ is the ideal gas constant, } \Delta H_f = 41 \pm 4 \text{ kJ/mol, } \Delta S_f = 0.10 \pm 0.01 \text{ kJ/mol-K}$$

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{OW}$:

5.18 (RP-TLC-k correlation, Bruggeman et al. 1982; Bruggeman et al. 1984)
5.16 (generator column-GC/ECD, Miller et al. 1984, 1985)
5.03 (calculated-TSA, Burkhard 1984)
4.67; 5.30 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
5.01, 5.10, 5.19, 5.10 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
5.13 (HPLC-k correlation, Noegrohati & Hammers 1992)
5.10 (recommended, Sangster 1993)
5.16 (recommended, Hensch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

8.37, 7.40; 7.33(0, 20°C, multi-column GC-k correlation; calculated at 20°C, Zhang et al. 1999)
7.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.68 (goldfish, 3% lipid by wt., static fish-water equilibration system, 23-d exposure, Bruggeman et al. 1981)
5.45 (goldfish, 10% lipid dry wt. in food, Bruggeman et al. 1981)
5.72 (guppy, 3.5% lipid by wt., Bruggeman et al. 1982, 1984)
4.14; 3.90 (goldfish, expl.; correlated, Mackay & Hughes 1984)
3.38–4.11 mean 4.00 (rainbow trout, 15°C, steady-state BCF, 7- to 96-d study, Oliver & Niimi 1985)
4.0 (rainbow trout, mean of 7–96 d exposure, Oliver & Niimi 1985)
4.53, 4.00 (rainbow trout: kinetic BCF; steady state BCF, Oliver & Niimi 1985)
4.26 (guppy, Gobas et al. 1987)
5.68 (goldfish, Noegrohati & Hammers 1992)
3.89; 3.42 (zebrafish: log BCF of wet wt basis; log BCF of lipid wt basis, Fox et al. 1994)
4.0, 5.09 (rainbow trout, flow through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.89, 5.43 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.00; 4.13 (Oncorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log $K_{OC}$:

4.83 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
4.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants $k = (0.024–0.038) \text{ min}^{-1}$ with $t_{1/2} = 18–29 \text{ min}$, $k = (0.033–0.048) \text{ min}^{-1}$ with $t_{1/2} = 14–21 \text{ min}$ and $k = (0.13–0.14) \text{ min}^{-1}$ with $t_{1/2} = 5 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; rate constant $k = (0.056–0.064) \text{ min}^{-1}$ with $t_{1/2} = 11–12 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; rate constant $k = (0.015–0.027) \text{ min}^{-1}$ with $t_{1/2} = 26–47 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)
tropospheric lifetime $\tau_{\text{calc}} = 8\text{–}17$ d for dichlorobiphenyls, based on $k_{\text{OH}}(\text{calc.}) = (1.4 \text{–} 2.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

Hydrolysis:

Biodegradation: 95% degradation at 24 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 920$ d$^{-1}$; $k_2 = 0.066$ d$^{-1}$ (23°C, goldfish, 3% lipid, Bruggeman et al. 1981; quoted, Waid 1986)
- $k_1 = 0.008$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
- $k_1 = 190$ d$^{-1}$; $k_2 = 0.11$ d$^{-1}$ (guppy, Bruggeman et al. 1984; quoted, Clark et al. 1990)
- $k_1 = 0.066$, $0.0523$ d$^{-1}$ (goldfish, exppt., calculated, Mackay & Hughes 1984)
- $k_1 = 280$ d$^{-1}$; $k_2 = 0.0082$ d$^{-1}$ (rainbow trout, Oliver & Niimi 1985)
- $k_1 = 38.3$, 49.2 h$^{-1}$; $1/k_2 = 360$, 220 h (goldfish, guppy, quoted, Hawker & Connell 1985)
- $k_1 = 1200$ d$^{-1}$ (guppy, Opperhuizen 1986)
- $k_1 = 122$ d$^{-1}$; $k_2 = 0.0089$ d$^{-1}$ (rainbow trout, calculated, Gobas & Mackay 1987)
- $k_1 = 2.96$, 3.07 d$^{-1}$; $\log 1/k_2 = 0.96$, 1.18 d (fish, quoted, Connell & Hawker 1988)
- $\log 1/k_2 = 2.1$, 2.3 h (fish, quoted, calculated-$K_{\text{OW}}$, Hawker & Connell 1988b)
- $\log k_2 = -0.96$, -1.17 d$^{-1}$ (fish, quoted, Thomann 1989)
- $k_1 = 2760$ d$^{-1}$; $k_2 = 0.368$ d$^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)
- $k_1 = 0.004$ d$^{-1}$ with $t_{\text{eq}} = 192$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005$ d$^{-1}$ with $t_{\text{eq}} = 149$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water:

- $t_{\text{eq}} = 18$–29 min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; $t_{\text{eq}} = 11$–12 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; $t_{\text{eq}} = 26$–47 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: clearance $t_{\text{eq}} = 10$ d in goldfish (Bruggeman et al. 1981)

- $t_{\text{eq}} = 6.5$ d in guppy (Bruggeman et al. 1984);
- $t_{\text{eq}} = 85$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and its muscle, $t_{\text{eq}} = 56$ d (Niimi & Oliver 1983).

Depuration $t_{\text{eq}} = 192$ d for high-dose treatment, $t_{\text{eq}} = 149$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.10 2,6-Dichlorobiphenyl (PCB-10)

![Chemical Structure](image)

**Common Name:** 2,6-Dichlorobiphenyl  
**Synonym:** PCB-10, 2,6-dichloro-1,1′-biphenyl  
**Chemical Name:** 2, 6-dichlorobiphenyl  
**CAS Registry No:** 33146-45-1  
**Molecular Formula:** C_{12}H_{8}Cl_{2}  
**Molecular Weight:** 223.098  
**Melting Point (°C):** 35.5 (Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 226.4 (calculated-Le Bas method at normal boiling point)  
185.8 (Ruelle & Kesselring 1997)  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):** 12.6 (differential scanning calorimetry, Miller et al. 1984)  
**Entropy of Fusion, ΔS_{fus} (J/mol K):** 41.0 (Miller et al. 1984)  
**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.789 (mp at 35.5°C)  
0.801 (Shiu & Mackay 1986)  
**Water Solubility (g/m³ or mg/L at 25°C):** 1.452 (shake flask-GC, Chiou et al. 1977)  
1.390 (generator column-GC/ECD, Miller et al. 1984,1985)  
0.294, 0.435, 0.245, 0.406 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
2.41 (generator column-GC/ECD, Dunnivant & Elzerman 1988)  
0.540 (generator column-GC/ECD, Opperhuizen et al. 1988)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):** 0.288 (GC-RI correlation, Burkhard et al. 1985a)  
0.365 (supercooled liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)  
0.336, 0.371 (supercooled P_{L}, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)  
0.347 (supercooled liquid P_{L}, GC-RI correlation, Fischer et al. 1992)  
log (P_{L}/Pa) = −3642/(T/K) + 11.74 (supercooled liquid P_{L}, GC-RT correlation, Falconer & Bidleman 1994)  
**Henry’s Law Constant (Pa m³/mol at 25°C):** 47.83 (calculated-P/C, Burkhard et al. 1985b)  
47.61 (calculated-MCI χ, Sabljic & Güsten 1989)  
23.30 (wetted wall column-GC, Brunner et al. 1990)  
42.86 (calculated-QSPR, Dunnivant et al. 1992)  
27.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 42 ± 6 kJ/mol, ΔS_{f} = 0.10 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.30 (quoted, Kaiser 1983)
4.96 (calculated-TSA, Burkhard 1984)
5.31 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.93 (generator column-GC/ECD, Miller et al. 1984, 1985)
4.97, 5.00, 4.97, 5.01 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.982 ± 0.013 (shake flask/slow stripping-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
4.99 (recommended, Sangster 1993)
4.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

7.18 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = – 4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
6.18 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

4.76 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
3.99 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $k = 0.043 \text{ min}^{-1}$ with $t_{1/2} = 16 \text{ min}$, $k = 0.082 \text{ min}^{-1}$ with $t_{1/2} = 8 \text{ min}$ and $k = 0.30 \text{ min}^{-1}$ with $t_{1/2} = 2 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; rate constants $k = 0.034 \text{ min}^{-1}$ with $t_{1/2} = 20 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; rate constants $k = 0.052 \text{ min}^{-1}$ with $t_{1/2} = 13 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8–17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc}) = (1.4 – 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 3.4–7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 – 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the $k_{OH}(\text{calc}) = (1.4 – 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism Alcaligenes eutrophus H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 183 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expn.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 93 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expn.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

© 2006 by Taylor & Francis Group, LLC
Surface water: $t_{1/2} = 16$ min, 8 min and 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; $t_{1/2} = 20$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; $t_{1/2} = 13$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 56$ d for high-dose treatment, $t_{1/2} = 53$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.11 3,3'-Dichlorobiphenyl (PCB-11)

Common Name: 3,3'-Dichlorobiphenyl
Synonym: PCB-11, 3,3'-dichloro-1,1'-biphenyl
Chemical Name: 3,3'-dichlorobiphenyl
CAS Registry No: 2050-67-1
Molecular Formula: C_{12}H_{8}Cl_{2}
Molecular Weight: 223.098
Melting Point (°C):
  29  (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
  320  (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
  226.4  (calculated-Le Bas method at normal boiling point)
  185.8  (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
  0.912  (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C):
  1.057  (supercooled liquid $S_L$, calculated-TSA, Burkhard et al. 1985b)
  0.0406, 0.102, 0.093, 0.0974 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  0.354  (generator column-GC/ECD, Dunnivant & Elzerman 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.0267  (P$_S$ from GC-RT correlation, Westcott & Bidleman 1981; Westcott et al. 1981)
  0.0865, 0.0952  (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Bidleman 1984)
  0.0645  (supercooled liquid P$_L$, GC-RT correlation, Burkhard 1984)
  0.0612  (GC-RI correlation, Burkhard et al. 1985a)
  0.0646  (supercooled liquid P$_L$, GC-RI correlation, Burkhard et al. 1985b)
  0.091, 0.076  (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  0.090  (selected P$_L$, supercooled liquid, Shiu & Mackay 1986)
  log (P$_P$/Pa) = − 3936/(T/K) + 12.14; 0.0306–0.143; 0.0646–0.0953 (literature. P$_S$ range; literature P$_L$ range, Delle & Site 1997)
Henry’s Law Constant (Pa m³/mol at 25°C):
  13.58  (calculated-P/C, Burkhard et al. 1985b)
  23.61  (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
  23.61; 38.69 (quoted explt.; calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
  23.61; 29.42 (quoted explt.; calculated-QSPR, Dunnivant et al. 1992)
  20.3  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  ln K$_{AW}$ = − $\Delta H_{AW}$/RT + $\Delta S_{AW}$/R; R is the ideal gas constant, $\Delta H_{AW}$ = 54 ± 3 kJ/mol, $\Delta S_{AW}$ = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K$_{OW}$:
  5.30 ± 0.1  (shake flask-GC/ECD, Bruggeman et al. 1982)
  5.34  (RP-TLC-$k'$ correlation, Bruggeman et al. 1982)
5.30, 5.39, 5.22, 5.18 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
5.27 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
7.86, 7.90; 7.93 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
4.90 (suspended particulate matter, calculated-$K_{OW}$ Burkhard 1984)
4.00 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ as as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = 2.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(calc) = 8–17$ d for dichlorobiphenyls, based on $k_{OH}(calc.) = (1.4 – 2.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

$k_{OH} = (4.1 \pm 1.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 ± 2 K (relative rate method, Kwok et al. 1995)

tropospheric lifetime $\tau(calc) = 3.4–7.2$ d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(exptl) = (2.0 – 4.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and the calculated $k_{OH}(calc) = (1.4 – 3.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2: 0.1385$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995)

Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{1/2} = 5$ d in rainbow trout, and $t_{1/2} < 5$ d in its muscle (Niimi & Oliver 1983)
7.1.1.12 3,4-Dichlorobiphenyl (PCB-12)

Common Name: 3,4-Dichlorobiphenyl
Synonym: PCB-12, 3,4-dichloro-1,1′-biphenyl
Chemical Name: 3,4-dichlorobiphenyl
CAS Registry No: 2974-92-7
Molecular Formula: C₁₂H₈Cl₂
Molecular Weight: 223.098

Melting Point (°C): 49–50 (Weingarten 1961)
Boiling Point (°C): 195–200 (Weast 1972–73)
Density (g/cm³):

Molar Volume (cm³/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), \( F \):
0.566 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
1.233 (calculated-TSA, supercooled liquid \( P_L \), Burkhard et al. 1985b)
0.0523, 0.112, 0.0888, 0.128 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00791 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0138 (supercooled liquid \( P_L \), calculated-mp, Dunnivant & Elzerman 1988)
0.280 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.091; 0.658 (quoted average of Brodsky & Ballschmiter 1988; calculated- \( \chi \), Patil 1991)
0.4004 (calculated-QSPR, Dunnivant et al. 1992)
0.930 (calculated-group contribution, Kühne et al. 1995)
0.268, 0.722 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
2.373 (calculated-mp and \( K_{OW} \), Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0532 (supercooled liquid \( P_L \), GT-RT correlation, Burkhard 1984)
0.0313 (GC-RI correlation, Burkhard et al. 1985a)
0.0532 (supercooled liquid \( P_L \), GC-RT correlation, Burkhard et al. 1985b)
0.078, 0.062 (supercooled liquid \( P_L \), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.741 (supercooled liquid \( P_L \), GC-RI correlation, Fischer et al. 1992)
\[ \log (P/P_{L}) = -3885/(T/K) + 11.92 \] (supercooled liquid \( P_L \), GC-RT correlation, Falconer & Bidleman 1994)
0.000736–0.0888; 0.0128–0.0783 (literature \( P_S \) range; literature \( P_L \) range, Delle Site 1997)
0.259 (\( P_L \), calculated-MCI \( \chi \) and Characteristic Root Index [CRI], Saçan & Balçıoğlu 1998)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\[ \ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; \] R is the ideal gas constant, \( \Delta H_{f} = 54 \pm 3 \text{ kJ/mol}, \Delta S_{f} = 0.14 \pm 0.01 \text{ kJ/mol·K} \) (Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Henry’s Law Constant (Pa m³/mol at 25°C):
20.77 (batch stripping/GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
14.18 (wetted-wall column-GC, Brunner et al. 1990)

Octanol/Water Partition Coefficient, log $K_{ow}$:
5.51 (Hansch & Leo 1979)
5.10, 5.51 (HPLC-RT correlation, calculated-$\pi$, Woodburn 1982; Woodburn et al. 1984)
5.29 (generator column-GC, Woodburn et al. 1984)
5.29 (generator column-GC/ECD, Doucette & Andren 1987)
5.26, 5.39, 5.22, 5.18 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
5.12 (HPLC-$k'$ correlation, Noegrohati & Hammers 1992)
5.29 (recommended, Sangster 1993)
5.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:
8.71, 7.80; 8.06(0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{oc}$:
4.85 (suspended particulate matter, calculated-$K_{ow}$, Burkhard 1984)
3.98 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: rate constants $k = (0.019–0.034)$ min⁻¹ with $t_{1/2} = 21–36$ min, $k = (0.041–0.064)$ min⁻¹ with $t_{1/2} = 11–17$ min and $k = (0.12–0.16)$ min⁻¹ with $t_{1/2} = 4–6$ min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO₂, respectively; rate constants $k = (0.013–0.029)$ min⁻¹ with $t_{1/2} = 26–52$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO₂ (Huang et al. 1996).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference: $k_{OH}$(calc.) = $1.8 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau$(calc) = 8–17 d for dichlorobiphenyls, based on $k_{OH}$(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for dichlorobiphenyls at room temp. (Atkinson 1987)

Hydrolysis:

Biodegradation: 100% degraded by Nocardia strain NCIB 10603 within one week (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 0.008$ d⁻¹ with $t_{1/2} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expn.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.010$ d⁻¹ with $t_{1/2} = 67$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expn.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the
experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 21–36$ min, 11–17 min and 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; $t_{1/2} = 26–52$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 88$ d for high-dose treatment, $t_{1/2} = 67$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.13 3,4′-Dichlorobiphenyl (PCB-13)

Common Name: 3,4′-Dichlorobiphenyl  
Synonym: PCB-13, 3,4′-dichloro-1,1′-biphenyl  
Chemical Name: 3,4′-dichlorobiphenyl  
CAS Registry No: 2974-90-5  
Molecular Formula: C_{12}H_8Cl_2  
Molecular Weight: 233.1

Melting Point (°C):  
51 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):  
1.084 (supercooled liquid S_L, Burkhard et al. 1985a)  
0.093 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)  
0.369 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
0.0572 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.0595 (GC-R1 correlation, Burkhard et al. 1985b)  
0.083, 0.067 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
log (P_L/P_a) = – 3885/(T/K) + 11.92 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol):  
12.36 (calculated-P/C, Burkhard et al. 1985b)  
31.92 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)  
25.75 (calculated-QSPR, Dunnivant et al. 1992)  
49.63 (calculated-QSPR, Achman et al. 1993)  
7.44 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
21.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
ln K_{AW} = – ΔH_{fus}RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 51 ± 25 kJ/mol, ΔS_{fus} = 0.13 ± 0.09 kJ/mol·K  
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:  
5.10 (calculated-TSA, Burkhard 1984)  
5.15 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)  
5.29 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)  
5.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{oa}:  
7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{bi}:
Sorption Partition Coefficient, \( \log K_{\text{OC}} \):

4.90  
(suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference: \( k_{\text{OH}}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (SAR, Atkinson 1987)

- Troospheric lifetime \( \tau(\text{calc}) = 8–17 \text{ d for dichlorobiphenyls, based on } k_{\text{OH}}(\text{calc}) = (1.4 – 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for dichlorobiphenyls at room temp. (Atkinson 1987)
- Troospheric lifetime \( \tau(\text{calc}) = 3.4–7.2 \text{ d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction } k_{\text{OH}}(\text{exptl}) = (2.0 – 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), and the calculated \( k_{\text{OH}}(\text{calc}) = (1.4 – 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
### 7.1.1.14 3,5-Dichlorobiphenyl (PCB-14)

![Chemical Structure](image)

**Common Name:** 3,5-Dichlorobiphenyl  
**Synonym:** PCB-14, 3,5-dichloro-1,1′-biphenyl  
**Chemical Name:** 3,5-dichlorobiphenyl  
**CAS Registry No:** 34883-41-5  
**Molecular Formula:** C\(_{12}\)H\(_8\)Cl\(_2\)  
**Molecular Weight:** 223.098

**Melting Point:** 36 °C (Hinkel & Hay 1928)  
**Boiling Point:** 31–32 °C (Weingarten 1961; Hutzinger et al. 1974)

**Density (g/cm\(^3\)):** 226.4 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, Δ\(H_{\text{fus}}\) (kJ/mol):**

**Entropy of Fusion, Δ\(S_{\text{fus}}\) (J/mol K):**

**Fugacity Ratio at 25°C (assuming Δ\(S_{\text{fus}} = 56\) J/mol K), F:** 0.872 (Shiu & Mackay 1986)

**Water Solubility (g/m\(^3\) or mg/L at 25°C):**

1.05 (supercooled liquid \(S_L\), calculated-TSA, Burkhard et al. 1985b)  
0.00792, 0.0425, 0.0722, 0.109 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**

0.128, 0.0662, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI \(\chi\), Burkhard et al. 1985a)  
0.0785 (supercooled liquid \(P_L\), GC-RI correlation, Burkhard et al. 1985b)  
0.126, 0.117 (supercooled \(P_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
\[\log (P_0/P) = -3885/(T/K) + 12.13\] (supercooled liquid \(P_L\), GC-RT correlation, Falconer & Bidleman 1994)

**Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):**

16.72 (calculated-P/C, Burkhard et al. 1985b)  
49.55 (calculated- QSAR-MCI \(\chi\), Sabljic & Güsten 1989)  
42.63 (calculated-QSPR, Dunnivant et al. 1992)  
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[\ln K_{\text{AW}} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R; R \text{ is the ideal gas constant, } \Delta H_{\text{f}} = 54 \pm 3 \text{ kJ/mol, } \Delta S_{\text{f}} = 0.14 \pm 0.01 \text{ kJ/mol-K}\] (Bamford et al. 2002)—see Comment by Goss et al. 2004

**Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):**

5.37 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)  
5.63, 5.56, 5.29, 5.16 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
5.28 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)  
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)  
5.41 (recommended, Sangster 1993)

**Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\) at 25°C or as indicated:**

8.82, 7.78 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)  
7.53 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF at 25°C or as indicated:
3.38–3.83 mean 3.79 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
3.82; 3.79 (rainbow trout: kinetic BCF, steady-state BCF, Oliver & Niimi 1985)

Sorption Partition Coefficient, log K_{oc}:
4.90 (suspended particulate matter, calculated-K_{ow}, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8–17$ d for dichlorobiphenyls, based on $k_{OH}(\text{calc}) = (1.4 - 2.9) \times 10^{-12}$

$\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987)

$k_{OH} = (4.2 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2$ K (relative rate method, Kwok et al. 1995)

tropospheric lifetime $\tau(\text{calc}) = 3.4–7.2$ d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{expt}) = (2.0 – 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated

$k_{OH}(\text{calc}) = (1.4 – 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 310 \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$log 1/k_2 = 1.3, 2.5$ h (fish, selected, calculated-$K_{ow}$, Hawker & Connell 1988)

$1/k_2 = 21.7$ d (rainbow trout, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-

phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_\frac{1}{2} = 15$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985),

$t_\frac{1}{2} = 14$ d in its muscle (Niimi & Oliver 1983).
7.1.1.15 4,4′-Dichlorobiphenyl (PCB-15)

Common Name: 4,4′-Dichlorobiphenyl  
Synonym: PCB-15, 4,4′-dichloro-1,1′-biphenyl  
Chemical Name: 4,4′-dichlorobiphenyl  
CAS Registry No: 2050-68-2  
Molecular Formula: C₁₂H₈Cl₂  
Molecular Weight: 223.098  
Melting Point (°C):  
149.3 (Lide 2003)  
Boiling Point (°C):  
317 (Lide 2003)  
Density (g/cm³ at 20°C): 1.0536  
Molar Volume (cm³/mol):  
226.4 (calculated-Le Bas method at normal boiling point)  
185.8 (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):  
Entropy of Fusion, ΔSₘₚ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F:  
0.059 (Shiu & Mackay 1986)  
0.0546 (Gobas et al. 1987)  
Water Solubility (g/m³ or mg/L at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
0.050 (Webb 1970)  
0.060 (Hoover 1971)  
0.080 (shake flask-GC/ECD, Walnöfer et al. 1973; Hutzinger et al. 1974)  
0.056 (generator column-GC/ECD, Weil et al. 1974)  
0.062 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)  
0.046 (generator column-HPLC/UV, Billington 1982)  
0.065 (generator column-HPLC/UV, Huang 1983)  
0.058 (generator column-HPLC/UV, Billington et al. 1988)  
0.151, 0.0774, 0.0952, 0.07055 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)  
0.0363 (generator column-GC/ECD, Dunnivant & Elzerman 1988)  
0.057 ± 0.0021*(generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)  
ln x = −2.8677 − 4839.46/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)  
1.116, 0.959 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)  
log S_l/(mol m⁻³) = − 807/(T/K) + 0.41 (supercooled liquid, linear regression of literature data, Li et al. 2003)  
log S_l/(mol m⁻³) = − 909/(T/K) + 0.68 (supercooled liquid, final adjusted eq., Li et al. 2003)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):  
0.00253* (Knudsen-effusion technique, extrapolated, Smith et al. 1964)  
0.043 (Pᵥ calculated from Pₘ using fugacity ratio F, Smith et al. 1964)  
0.071, 0.084 (supercooled liquid Pᵥ, GC-RT correlation, different stationary phases, Bidleman 1984)  
0.0508 (supercooled liquid Pᵥ, Burkhard 1984)  
0.075, 0.059 (supercooled Pᵥ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
0.00313 (GC-RI correlation, Burkhard et al. 1985a)  
0.0508 (supercooled liquid Pᵥ, GC-RI correlation, Burkhard et al. 1985b)  
0.0263 (extrapolated Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = −5416/(T/K) + 12.585; temp range 50–87°C (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 10.10 – 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)

log (PL/Pa) = −3971/(T/K) + 12.18; (supercooled liquid PL, GC-RT correlation, Falconer & Bidleman 1994)

log (PS/Pa) = −4977/(T/K) + 14.10; temp range –20 to 30°C (gas saturation-GC, solid, Wania et al. 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

30.4 (calculated-P/C, Murphy et al. 1983)
11.04 (calculated-P/C, Burkhard et al. 1985b)
14.69 (calculated, Coates & Elzerman 1986)
17.0 (calculated-P/C, Shi & Mackay 1986)
20.16 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
9.66 (wetted-wall column-GC/ECD, Fendinger & Glotfelty 1990)
18.95: 22.70 (quoted explt.; calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

14.12, 13.49 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m³/mol)] = −2921/(T/K) + 10.92 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{ow}:

5.58 (shake flask-GC, Chiu et al. 1977)
5.17 (HPLC-RT correlation, Sugiura et al. 1978)
5.51 (Hansch & Leo 1979)
5.50 (shake flask-GC, Platford 1982)
5.36 ± 0.1; 5.28 (shake flask-GC; RP-TLC-k’ correlation, Bruggeman et al. 1982)
4.92 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
5.33 (generator column-GC/ECD; Woodburn et al. 1984)
4.82 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.30 (selected, Shi & Mackay 1986)
5.33 (generator column-GC/ECD, Doucette & Andren 1987)
5.03, 5.39, 5.22, 5.28 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
5.23 (recommended, Sangster 1993)
5.58 (recommended, Hansch et al. 1995)
5.35, 5.36 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{oa} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.67* (generator column-GC, measured range – 10 to 20°C, Harner & Mackay 1995)
log K_{oa} = −5.10 + 3791.7/(T/K), temp range: −10 to 20°C (generator column-GC, Harner & Mackay 1995)
7.88 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{oa} = −5.06 + 3792/(T/K), (temp range – 10 to + 20°C, Harner & Bidleman 1996)
8.87, 7.88; 7.89 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
Polychlorinated Biphenyls (PCBs)

8.12 \( (\text{calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002}) \)

7.73; 7.77 \( (\text{calibrated GC-RT correlation, GC-RT correlation, Wania et al. 2002}) \)

7.65, 7.85 \( (\text{LDV literature derived value, FAV final adjusted value, Li et al. 2003}) \)

\( \log K_{OA} = \frac{4078}{(T/K)} - 5.83 \) \( (\text{FAV final adjusted eq., Li et al. 2003}) \)

Bioconcentration Factor, log BCF:

2.97 \( \text{(killifish, Goto et al. 1978)} \)

2.33 \( \text{(fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)} \)

3.47 \( \text{(calculated-S, Kenaga 1980)} \)

3.58 \( \text{(rainbow trout, highest value-non-equilibrated, Oliver & Niimi 1984)} \)

4.27 \( \text{(<Picea omorika>, Reischl et al. 1989 from Reischl 1988)} \)

4.06, 5.36 \( \text{(fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)} \)

Sorption Partition Coefficient, log \( K_{OC} \):

4.30 \( \text{(calculated-solubility, Kenaga 1980)} \)

4.91 \( \text{(suspended particulate matter, calculated-} K_{OW}, \text{ Burkhard 1984)} \)

5.65 \( \text{(EPA-B2 river sediment, Coates & Elzerman 1986)} \)

4.03 \( \text{(soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)} \)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization: estimated evaporation \( t_{1/2} = 4.5 \) h for an initial concentration of 0.03 ppm in a 4.5 cm depth of water solution in a glass dish and \( t_{1/2} = 1.7 \) h with stirring of the solution; while experimental observed \( t_{1/2} = 4.0 \) h and 1.5 h under the same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with \( NO_3 \) radical and \( k_{O3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference: \( k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (SAR, Atkinson 1987)

Tropospheric lifetime \( \tau(\text{calc}) = 8–17 \) d for dichlorobiphenyls, based on \( k_{OH}(\text{calc}) = (1.4 – 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for dichlorobiphenyls at room temp. (Atkinson 1987)

Tropospheric lifetime \( \tau(\text{calc}) = 3.4–7.2 \) d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction \( k_{OH}(\text{exptl}) = (2.0 – 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), and the calculated \( k_{OH}(\text{calc}) = (1.4 – 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% biodegraded by \textit{Alcaligenes} sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

\( t_{1/2} = 72 \) h for 50% degradation in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, and 55% degradation at 24 h in another PCB mixture by microorganism \textit{Alcaligenes eutrophus} H850 (Bedard et al. 1986);

Aerobic biodegradation \( t_{1/2} = 1.42 \) d without the addition of polymer chitin, \( t_{1/2} = 0.98 \) d with chitin and \( t_{1/2} = 0.46 \) d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\( k_2 = 0.009 \text{ d}^{-1} \) with \( t_{1/2} = 81 \) d \( (8^\circ \text{C}, \text{juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.)} \) \( - \) high-dose treatment, Buckman et al. 2004)

\( k_2 = 0.007 \text{ d}^{-1} \) with \( t_{1/2} = 99 \) d \( (8^\circ \text{C}, \text{juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.)} \) \( - \) high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{1/2} = 57.5$ d in Lake Michigan, 57.5 d (Neely 1983); 
aerobic biodegradation $t_{1/2} = 1.42$ d without the addition of polymer chitin, $t_{1/2} = 0.98$ d with chitin 
and $t_{1/2} = 0.46$ d with chitin plus adapted microbes in flow microcosm systems with water and 
sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:
Sediment:
Soil:
Biota: $t_{1/2} = 27$ d in *Picea omorika* (Reischl et al. 1989).

depuration $t_{1/2} = 81$ d for high-dose treatment, $t_{1/2} = 99$ d for high-dose + enzyme CYPIA-inducing 
compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

### TABLE 7.1.1.15.1
Reported aqueous solubilities, vapor pressure and octanol-air partition coefficients of 4,4’-dichlorobiphenyl 
(PCB-15) at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
<td>$P/Pa$</td>
</tr>
<tr>
<td>5</td>
<td>0.021</td>
<td>29.88</td>
<td>0.149</td>
</tr>
<tr>
<td>15</td>
<td>0.0346</td>
<td>29.88</td>
<td>0.152</td>
</tr>
<tr>
<td>25</td>
<td>0.0570</td>
<td>66.58</td>
<td>0.504</td>
</tr>
<tr>
<td>35</td>
<td>0.106</td>
<td>66.58</td>
<td>0.432</td>
</tr>
<tr>
<td>45</td>
<td>0.186</td>
<td>76.78</td>
<td>1.26</td>
</tr>
<tr>
<td></td>
<td></td>
<td>76.78</td>
<td>1.27</td>
</tr>
<tr>
<td></td>
<td></td>
<td>87.0</td>
<td>3.55</td>
</tr>
<tr>
<td></td>
<td></td>
<td>87.0</td>
<td>3.57</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}/(kJ \ mol^{-1}) = 40.2$ 
at 5–45°C

$log P/mmHg = A \times B/(T/K)$ 

$A = 13.460$ 

$B = 5416$ 

$\Delta H_{subl}/(kJ \ mol^{-1}) = 95.3$

$\Delta H_{vap}/(kJ \ mol^{-1}) = 40.2$

$\Delta H_{res}/(kJ \ mol^{-1}) = 72.6$

$log K_{OA} = A \times B/T$

$A = 14.10$ 

$B = 4977$
FIGURE 7.1.1.15.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 4,4'-dichlorobiphenyl (PCB-15).
7.1.1.16 2,2′,3-Trichlorobiphenyl (PCB-16)

Common Name: 2,2′,3-Trichlorobiphenyl
Synonym: PCB-16, 2,2′,3-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,3-trichlorobiphenyl
CAS Registry No: 38444-78-9
Molecular Formula: C₁₂H₇Cl₃
Molecular Weight: 257.543
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
  - 247.3 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH₉₃ (kJ/mol):
Entropy of Fusion, ΔS₉₃ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉₃ = 56 J/mol K), F:
  - 0.934 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  - 0.505 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
  - 0.293 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
  - 0.205 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
  - 0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)
  - 0.174 (calculated-MCI χ, Patil 1991)
  - 0.674 (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  - 0.0522, 0.066, 0.033 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
  - 0.069 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
  - 0.0383, 0.060 (supercooled Pₐ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  - 0.0275 (20°C, supercooled liquid Pₐ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.10 – 4100/(T/K) (GC-RT correlation, Tateya et al. 1988)
  - 0.0427; 0.0427 (supercooled liquid Pₐ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  - 0.0506; 0.0427 (Pₐ, calculated-MCI χ and Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
  - 35.16 (calculated-P/C, Burkhard et al. 1985b)
  - 80.0 (calculated-P/C, Shiu & Mackay 1986)
  - 24.11 (20°C, calculated-P/C, Murphy et al. 1987)
  - 81.77 (batch stripping, Atlas et al. 1982)
  - 20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
  - 25.45 (calculated-QSPR, Dunnivant et al. 1992)
  - 4.02, 11.74 (0, 15°C, from modified two-film exchange model, Hornbükle et al. 1994)
  - 9.36 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  - 25.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
\[ \ln K_{\text{AW}} = -\frac{\Delta H_f}{RT} + \frac{\Delta S_f}{R}; \text{ R is the ideal gas constant, } \Delta H_f = 47 \pm 24 \text{ kJ/mol, } \Delta S_f = 0.12 \pm 0.08 \text{ kJ/mol-K} \] (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):

- 5.36 (calculated-TSA, Burkhard 1984)
- 4.15 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.31 (calculated-\( \pi \) const., Rapaport & Eisenreich 1984)
- 5.12 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
- 5.12 (recommended, Sangster 1993)
- 5.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \( \log K_{\text{OA}} \) or as indicated and reported temperature dependence equations:

- 7.22, 7.18 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- \( \log K_{\text{OA}} = -6.50 + 4240/(T/K) \) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.87, 7.98 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 7.32 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{\text{OC}} \):

- 5.16 (suspended particulate matter, Burkhard 1984)
- 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.00 (soil, calculated-\( K_{\text{OW}} \), Girvin & Scott 1997)

Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

Volatilization:

Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO3}} \) with NO3 radical and \( k_{\text{O3}} \) with O3 or as indicated, *data at other temperatures see reference:

- \( k_{\text{OH}}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for trichlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 14 - 30 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
- \( k_{\text{OH}}(\text{aq}) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \), PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from \( t_{1/2} \approx 4 - 11 \text{ d} \) in freshwater systems, \( t_{1/2} = 0.1 - 10 \text{ d} \) in cloud water, \( t_{1/2} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- \( k_{\text{OH}}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for trichlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 6.9 - 15 \text{ d} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degraded by Nocardia strain NCIB 10603 within 7 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

- \( k_2 = 0.008 \text{ d}^{-1} \) with \( t_{1/2} = 90 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.010 \text{ d}^{-1} \) with \( t_{1/2} = 72 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 90$ d for high-dose treatment, $t_{1/2} = 72$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.17  2,2',4-Trichlorobiphenyl (PCB-17)

![Chemical Structure]

Common Name: 2,2',4-Trichlorobiphenyl  
Synonym: PCB-17, 2,2',4-trichloro-1,1'-biphenyl  
Chemical Name: 2,2',4-trichlorobiphenyl  
CAS Registry No: 37680-66-3  
Molecular Formula: C_{12}H_{8}C_{2}  
Molecular Weight: 257.543  
Melting Point (°C):  
35  (estimated, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm³):  
247.3  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
0.292  (supercooled liquid $S_L$, Burkhard et al. 1985a)  
0.259  (supercooled liquid $S_L$, Murphy et al. 1987)  
0.103  (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)  
0.647  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
0.080  (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.0566, 0.0828, 0.0219  (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)  
0.0705, 0.0739  (supercooled $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
0.0335  (supercooled liquid $P_L$, Murphy et al. 1987)  
0.0692; 0.0526  (supercooled liquid $P_L$: GC-RI correlation, different stationary phases, Fischer et al. 1992)  
log ($P_P/P_a$) = – 3935/(T/K) + 12.05  (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)  
0.0692; 0.526  (P_L, quoted lit.; calculated-MCI $\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
52.18  (calculated-P/C, Burkhard et al. 1985b)  
33.03  (calculated-P/C, Murphy et al. 1987)  
40.63  (calculated-molecular connectivity indices, Sablje & Güsten 1989)  
37.82  (calculated-QSPR, Dunnivant et al. 1992)  
26.04  (calculated-QSPR, Achman et al. 1993)  
13.9  (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
32.1  (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
ln $K_{AW} = \frac{-\Delta H_{RT} + \Delta S_{RT}}{R}$; R is the ideal gas constant, $\Delta H_{RT} = 39 \pm 21$ kJ/mol, $\Delta S_{RT} = 0.10 \pm 0.07$ kJ/mol·K  (Bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log $K_{OW}$:  
4.60, 5.76  (RP-HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenrich 1984)  
5.39  (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)  
5.50  (generator column-GC, Larsen et al. 1992)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

8.06; 7.74 (0; 20°C, multi-column GC-kr correlation, Zhang et al. 1999)
7.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

5.24 (suspended particulate matter, Burkhard 1984)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.84 (calculated-QSAR-MCI $\chi$, Sabljic et al. 1995)
5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}$(calc) = (0.7 – 1.6) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}$(aq.) = 7.5 × 10$^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_\frac{1}{2}$ ~ 4–11 d in freshwater systems, $t_\frac{1}{2}$ = 0.1–10 d in cloud water, $t_\frac{1}{2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}$(calc) = (1.0 – 2.1) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k$_1$ and k$_2$):

$k_2$ = 0.009 d$^{-1}$ with $t_\frac{1}{2}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2$ = 0.007 d$^{-1}$ with $t_\frac{1}{2}$ = 99 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_\frac{1}{2}$ ~ 4–11 d in freshwater systems, $t_\frac{1}{2}$ = 0.1–10 d in cloud water, $t_\frac{1}{2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Ground water:
Sediment:
Soil:
Biota: depuration $t_\frac{1}{2}$ = 81 d for high-dose treatment, $t_\frac{1}{2}$ = 99 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.18 2,2',5-Trichlorobiphenyl (PCB-18)

Common Name: 2,2',5-Trichlorobiphenyl
Synonym: PCB-18, 2,2',5-trichloro-1,1'-biphenyl
Chemical Name: 2,2',5-trichlorobiphenyl
CAS Registry No: 37680-65-2
Molecular Formula: C₁₂H₇Cl₃
Molecular Weight: 257.543
Melting Point (°C): 43–44 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.1485
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHₘ (kJ/mol):
Entropy of Fusion, ΔSₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘ = 56 J/mol K), F:
0.648 (Mackay et al. 1980)
0.651 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.640 (shake flask-GC/ECD, Weil et al. 1974)
0.248 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.016 (radioactive isotope-¹⁴C labeled, Metcalf et al. 1975)
0.0614 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
0.085 (Kenaga & Goring 1980; Kenaga 1980)
0.110 (shake flask GC/ECD, Bruggeman et al. 1981)
0.299 (20°C, supercooled liquid Sₗ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.203, 0.135, 0.100, 0.112 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
0.510; 0.780 (generator column-GC/ECD, supercooled liquid Sₗ, Dunnivant & Elzerman 1988)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.267 (Neely 1981)
0.412 (Pₛ calculated from Pₗ using fugacity ratio F, Neely 1981)
0.012 (Neely 1983)
0.0094 (supercooled liquid Pₗ, Burkhard 1984)
0.0605 (GC-RI correlation, Burkhard et al. 1985a)
0.0904 (supercooled liquid Pₗ, GC-RT correlation, Burkhard et al. 1985b)
0.0776, 0.0833 (supercooled Pₛ; GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.143; 0.220 (selected: solid Pₛ; supercooled liquid Pₗ, Shiu & Mackay 1986)
0.0352 (20°C, supercooled liquid Pₗ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
\[ \log (P_{/\text{mmHg}}) = 10.10 - 4090/(T/K) \] (GC-RT correlation, Tateya et al. 1988)
0.0603, 0.0851 (supercooled liquid Pₛ; GC-RI correlation, different stationary phases, Fischer et al. 1992)
\[ \log (Pₗ/Pa) = -3935/(T/K) + 12.09; \] (supercooled liquid Pₗ, GC-RT correlation, Falconer & Bidleman 1994)
0.033–0.0762; 0.035–0.116 (literature Pₛ range; literature Pₗ range, Delle Site 1997)
Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101.53 (23°C, gas stripping-GC, Atlas et al. 1982)
20.26 (20°C, gas stripping-GC, Oliver 1985)
38.5 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
25.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.11, 12.07, 17.64, 25.358* ± 0.34, 34.14 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)

\[ \ln K_{AW} = 9.5020 - 4197.74/(T/K); \text{ temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)} \]

\[ K_{AW} = \exp\left[-(34.9/\text{kJ·mol}^{-1}/R T) + (0.079/\text{kJ·mol}^{-1} \cdot \text{K}^{-1}/R)\right]; \text{ where } R = 8.314 \text{ J·K}^{-1}·\text{mol}^{-1} \text{ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)} \]

25.3 (exptl. data, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_m/RT + \Delta S_m/R; \text{ R is the ideal gas constant, } \Delta H_m = 35 \pm 3 \text{ kJ/mol, } \Delta S_m = 0.08 \pm 0.01 \text{ kJ/mol-K} \]

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

3.89 (radiolabeled-14C, Metcalf et al. 1975)
6.22 (shake flask, Hansch & Leo 1979)
5.88 (calculated after Rekker 1977, Königmann 1981)
5.64 (RP-TLC-k’ correlation, Bruggeman et al. 1982)
5.59; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn 1982)
4.39, 5.55 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.60; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
4.97 (HPLC-RT correlation, DeVoe et al. 1987)
4.97, 5.68 (HPLC-k’ correlation, De Cock & Lord, 1987)
5.60 (generator column-GC/ECD, Doucette & Andre 1987, 1988)
5.31, 5.37, 5.29, 5.37 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.55 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
5.44 (generator column-GC, Larsen et al. 1992)
5.44 (recommended, Sangster 1993)
5.60 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C or as indicated and reported temperature dependence equations:

7.60; 7.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

\[ \log K_{oa} = -6.00 + 4060/(T/K); \text{ temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)} \]

8.39 (10°C, estimated, Thomas et al. 1998)
8.70, 7.79 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
7.48 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log \( BCF \):

3.86, 3.76, 2.91, 3.81 (algae, snail, mosquito, fish, 14C-labeled, Metcalf et al. 1975)
1.72 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.39 (calculated-S, Kenaga 1980)
5.52; 5.83 (goldfish: 10% lipid by wt. in food; 3% lipid, static equilibration system-GC/ECD, 23-d exposure studies, Bruggeman et al. 1981)
3.43–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.91, 4.23; 5.77 (rainbow trout, laboratory data: kinetic BCF(k1/k2), steady-state BCF (Cp/Cw); Lake Ontario field BCF, Oliver & Niimi 1985)
4.30 (fish, calculated-Cp/Cw or k1/k2, Connell & Hawker 1988; Hawker 1990)
3.75 (Picea omorika, Reischl et al. 1989 from Reischl 1988)
4.23 (fish, Isnard & Lambert 1989)
5.82; 5.87 (goldfish; rainbow trout, Noegrohati & Hammers 1992)
4.11; 5.64 (zebrafish: log BCFw wet wt basis; log BCFw lipid wt basis, Fox et al. 1994)
Polychlorinated Biphenyls (PCBs)

2.60–4.19 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.08–6.01 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.23, 5.32 (rainbow trout, flow through-96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.40, 5.60 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.64 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:

- 4.50, 4.50, 5.0 (sediments: offshore Grand Haven 2.0% OC, nearshore Grand Haven 3.4% OC, Benton Harbor sediment 3.8% OC, batch equilibrium-sorption isotherm, Voice et al. 1983; Voice & Weber, Jr., 1985)
- 5.24 (suspended particulate matter, Burkhard 1984)
- 5.40; 5.50; 5.20(field data of sediment trap material; Niagara River-organic matter; calculated-$K_{OW}$ Oliver & Charlton 1984)
- 5.1–6.3, 5.5; 7.0(suspended sediment, average; algae > 50 µm, Oliver 1987a)
- 5.34 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 4.49 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 4.85, 4.15 (Aldrich humic acid substrate with methyl salicylate, organic polymers present in Huron River water, Chin et al. 1990)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.23 (soil, calculated-MCI, Sabljic et al. 1995)
- 4.53; 4.57 (soil, calculated-Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioglu 1996)
- 5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
- 4.85 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$\tau_{(calc)}$ = $(0.7 – 1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime

$\tau_{(calc)}$ = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$\tau_{(aq.)}$ = $6.9 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{1/2}$=4–11 d in freshwater systems, $t_{1/2}$ = 0.1–10 d in cloud water, $t_{1/2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

Hydrolysis:

Biodegradation: 50–80% being degraded by Alcaligenes sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1$ = 950 d$^{-1}$; $k_2$ = 0.048 d$^{-1}$ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)

$k_1$ = 0.0037 d$^{-1}$; $k_2$ = 0.048 d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark 1990)

$k_1$ = 0.048, 0.0372 d$^{-1}$ (goldfish, expl., correlated, Mackay & Hughes 1984)

$k_1$ = 300 d$^{-1}$; $k_2$ = 0.0037 d$^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1$ = 39.6 h$^{-1}$; $1/k_1$ = 500 h (goldfish, quoted, Hawker & Connell 1985)

$k_2$ = 0.292 d$^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)

$k_2$ = 0.020 d$^{-1}$ with $t_{1/2}$ = 36 d and $k_2$ = 0.029 d$^{-1}$ with $t_{1/2}$ = 24 d for food concn of 29 ng/g and 182 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: \( t_{1/2} = 43.1 \text{ d} \) in Lake Michigan (Neely 1983); \( t_{1/2} \sim 4–11 \text{ d} \) in freshwater systems, \( t_{1/2} = 0.1–10 \text{ d} \) in cloud water, \( t_{1/2} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991).

Groundwater:

Soil: Sorption-Desorption Rate Constants: release rate constants \( k_d \) for labile PCBs sorbed to utility substation soils are: \( 0.47 \text{ d}^{-1} \) from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, \( 1.16 \text{ d}^{-1} \) from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, \( 1.21 \text{ d}^{-1} \) from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.17 \text{ d}^{-1} \) from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants \( k_d \) for nonlabile PCBs sorbed to utility substation soils are; \( 0.00838 \text{ d}^{-1} \) from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, \( 0.00368 \text{ d}^{-1} \) from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, \( 0.00357 \text{ d}^{-1} \) from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00062 \text{ d}^{-1} \) from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: \( t_{1/2} = 190 \text{ d} \) in rainbow trout, 190 d and its muscle 86 d (Niimi & Oliver 1983);
\( t_{1/2} = 190 \text{ d} \) in fish (rainbow trout, Niimi & Oliver 1983; Oliver & Niimi 1985);
\( t_{1/2} = 26 \text{ d} \) in worms at 8°C (Oliver 1987c);
\( t_{1/2} = 25 \text{ d} \) in omorika (Reischl et al. 1989)

Depuration \( t_{1/2} = 32–42 \text{ d} \) for a 32-d dietary exposure followed by a 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

Depuration \( t_{1/2} = 79 \text{ d} \) for high-dose treatment, \( t_{1/2} = 96 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.19  2,2′,6-Trichlorobiphenyl (PCB-19)

Common Name: 2,2′,6-Trichlorobiphenyl
Synonym: PCB-19, 2,2′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,6-trichlorobiphenyl
CAS Registry No: 38444-73-4
Molecular Formula: C_{12}H_{7}Cl_{7}
Molecular Weight: 257.543
Melting Point (°C):
   46  (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
   247.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   0.345  (supercooled liquid S_{L}, Burkhard et al. 1985a)
   0.448  (supercooled liquid S_{L}, Murphy et al. 1987)
   0.447, 0.408, 0.235, 0.246  (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
   0.814  (calculated-TSA, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   0.167  (P_{L}, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
   0.171  (GC-RI correlation, Burkhard et al. 1985b)
   0.113, 0.131  (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
   0.0529  (supercooled liquid P_{L}, Murphy et al. 1987)
log (P/mmHg) = 9.86 – 3970/(T/K)  (GC-RT correlation, Tateya et al. 1988)
log (P_{L}/Pa) = – 3836/T + 11.93  (supercooled liquid P_{L}, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
   124.6  (calculated-P/C, Burkhard et al. 1985b)
   30.70  (calculated-P/C, Murphy et al. 1987)
   45.09  (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
   23.30  (wetted-wall column-GC, Brunner et al. 1990)
   44.74  (calculated-QSPR, Dunnivant et al. 1992)
   13.9  (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
   32.2  (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ΔH_{f}/RT + ΔS_{f}/R;  R is the ideal gas constant, ΔH_{f} = 39 ± 21 kJ/mol, ΔS_{f} = 0.10 ± 0.07 kJ/mol·K
(bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
   3.75, 5.48  (RP-HPLC correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
   4.88, 5.06, 5.03, 5.19  (RP-HPLC-k′ correction, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
Octanol/Air Partition Coefficient, log $K_{OA}$:

- 6.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

- 5.28 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.7 – 1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(calc) = (1.0 – 2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9–15$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 155$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.008$ d$^{-1}$ with $t_{1/2} = 84$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
  - tropospheric lifetime of 6.9–15 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 155$ d for high-dose treatment, $t_{1/2} = 84$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.20 2,3,3′-Trichlorobiphenyl (PCB-20)

Common Name: 2,3,3′-Trichlorobiphenyl
Synonym: PCB-20, 2,3,3′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,3′-trichlorobiphenyl
CAS Registry No: 38444-84-7
Molecular Formula: C_{12}H_7Cl_3
Molecular Weight: 257.543
Melting Point (°C):
58 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
337 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm³):
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.402 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.033 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.0283 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0269 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
log (P/mmHg) = 10.40 – 4310/(T/K), (GC-RT correlation, Tateya et al. 1988)
0.0302 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (PL/Pa) = – 4075/(T/K) + 12.12 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
Henry’ Law Constant (Pa m³/mol at 25°C):
81.77 (batch stripping-GC, Atlas et al. 1982)
17.23 (calculated-P/C, Burkhard et al. 1985b)
30.7 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
16.21 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.01 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
\ln K_{AW} = -\Delta H_{H}/RT + \Delta S_{H}/R; R is the ideal gas constant, \Delta H_{H} = 41 ± 4 kJ/mol, \Delta S_{H} = 0.10 ± 0.07 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
4.99, 5.57 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.57 (calculated-TSA, Hawker & Connell 1988a)
5.68 (generator column-GC, Larsen et al. 1992)
5.62 (recommended, Sangster 1993)
5.57 (recommended, Hansch et al. 1995)
5.4846 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$ or as indicated:

9.51, 8.49  (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
7.95  (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:

5.23  (suspended particulate matter, Burkhard 1984)
4.01–4.88; 5.20  (range, calculated from sequential desorption of 11 urban soils; lit. value, Krauss & Wilcke 2001)
5.13; 5.01, 4.88, 5.45 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH(\text{calc})} = (0.7 – 1.6) \times 10^{-12} $ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH(\text{calc})} = (1.0 – 2.1) \times 10^{-12} $ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9–15$ d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2 = 0.008$ d$^{-1}$ with $t_\frac{1}{2} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008$ d$^{-1}$ with $t_\frac{1}{2} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_\frac{1}{2} = 91$ d for high-dose treatment, $t_\frac{1}{2} = 88$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.21 2,3,4-Trichlorobiphenyl (PCB-21)

Common Name: 2,3,4-Trichlorobiphenyl
Synonym: PCB-21, 2,3,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4-trichlorobiphenyl
CAS Registry No: 55702-46-0
Molecular Formula: C₁₂H₇Cl₃
Molecular Weight: 257.543
Melting Point (°C):
101–102  (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
247.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.176 (mp at 102°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.469  (calculated-TSA, Burkhard et al. 1985b)
0.224, 0.195, 0.142; 0.132 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
0.103  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174  (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00489  (GC-RI correlation, Burkhard et al. 1985a)
0.0269  (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0295  (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_v/P_a) = – 4075/(T/K) + 12.11 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
14.79  (calculated-P/C, Burkhard et al. 1985b)
23.0  (calculated-QSPR, Dunnivant et al. 1992)
29.0  (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 41 ± 4 kJ/mol, ΔS_{fus} = 0.10 ± 0.02 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88  (calculated after Rekker 1977, Könemann 1981)
5.77  (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.51, 5.61, 5.87, 5.73 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
5.860 ± 0.017 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990;)
5.68  (recommended, Sangster 1993)
5.86  (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.16  (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$

5.19 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{\frac{1}{2}}$:

Volatilization:

Photolysis: rate constants $k = 0.021\; \text{min}^{-1}$ with $t_{\frac{1}{2}} = 33\; \text{min}$, $k = 0.059\; \text{min}^{-1}$ with $t_{\frac{1}{2}} = 12\; \text{min}$ and $t_{\frac{1}{2}} = 0.14\; \text{min}^{-1}$ with $t_{\frac{1}{2}} = 5\; \text{min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu$g/mL TiO$_2$, respectively; rate constants $k = 0.0050\; \text{min}^{-1}$ with $t_{\frac{1}{2}} = 139\; \text{min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu$g/mL TiO$_2$ (Huang et al. 1996)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.7 - 1.6) \times 10^{-12}\; \text{cm}^3\; \text{molecule}^{-1}\; \text{s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14 - 30\; \text{d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (1.0 - 2.1) \times 10^{-12}\; \text{cm}^3\; \text{molecule}^{-1}\; \text{s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9 - 15\; \text{d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{\frac{1}{2}} = 33\; \text{min}$, 12 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu$g/mL TiO$_2$, respectively; $t_{\frac{1}{2}} = 139\; \text{min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu$g/mL TiO$_2$ (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:
7.1.1.22 2,3,4′-Trichlorobiphenyl (PCB-22)

Common Name: 2,3,4′-Trichlorobiphenyl
Synonym: PCB-22, 2,3,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4′-trichlorobiphenyl
CAS Registry No: 38444-85-8
Molecular Formula: C₁₂H₇Cl₃
Molecular Weight: 257.543
Melting Point (°C):
73 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
69.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHᵥₐₜ (kJ/mol):
Entropy of Fusion, ΔSᵥₐₜ (J/mol K):
Fugacity Ratio at 25°C, F:
0.335 (calculated-assuming ΔSᵥₐₜ = 56 J/mol K, Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C):
0.397 (supercooled liquid Sᵥ,L, Burkhard et al. 1985b)
0.142 (supercooled liquid Sᵥ,L, Murphy et al. 1987)
0.408 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0696 (calculated-QSPR, Dunnivant et al. 1992)
0.187 (calculated-group contribution method, Kühne et al. 1995)
0.0677, 0.178 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.469 (calculated-mp and Kᵥₐₜ, Ran et al. 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0239 (Pᵥ,L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0084 (GC-RI correlation, Burkhard et al. 1985b)
0.026, 0.023 (supercooled liquid Pᵥ,L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0111 (supercooled liquid Pᵥ,L, Murphy et al. 1987)
0.0191, 0.0263 (supercooled liquid Pᵥ,L; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pᵥ,L/Pa) = – 4075/(T/K) + 12.08 (supercooled liquid Pᵥ,L, GC-RT correlation, Falconer & Bidleman 1994)
0.0478 (Pᵥ,L calculated-MCI χ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry’s Law Constant (Pa·m³/mol at 25°C):
15.40 (calculated-P/C, Burkhard et al. 1985b)
20.16 (calculated-P/C, Murphy et al. 1987)
14.18 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.60 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
25.03; 19.35 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
13.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
31.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln Kᵥₐₜ = – ΔHᵥₐₜ/RT + ΔSᵥₐₜ/R; R is the ideal gas constant, ΔHᵥₐₜ = 31 ± 1 kJ/mol, ΔSᵥₐₜ = 0.10 ± 0.07 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{ow}$:
- 4.84, 5.42 (RP-HPLC-k correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 5.29 (RP-HPLC-k correlation, Brodsky & Balischmiller 1988)
- 5.63 (generator column-GC, Larsen et al. 1992)
- 5.45 (recommended, Sangster 1993)
- 5.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:
- 9.60; 8.58 (0; 20°C, multi-column GC-k correlation, Zhang et al. 1999)
- 8.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$ or log $K_{bi}$:
Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
- 5.70, 4.90 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log $K_{oc}$:
- 5.24 (suspended particulate matter, Burkhard 1984)
- 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.90 (soil, calculated-$K_{ow}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}$(calc) = $(0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}$(aq.) = $7.4 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}$(calc) = $(1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.012$ d$^{-1}$ with $t_{1/2} = 56$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.011$ d$^{-1}$ with $t_{1/2} = 64$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
- Surface water: $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 56$ d for high-dose treatment, $t_{1/2} = 64$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

© 2006 by Taylor & Francis Group, LLC
7.1.1.23 2,3,5-Trichlorobiphenyl (PCB-23)

Common Name: 2,3,5-Trichlorobiphenyl
Synonym: PCB-23, 2,3,5-trichloro-1,1'-biphenyl
Chemical Name: 2,3,5-trichlorobiphenyl
CAS Registry No: 55720-44-0
Molecular Formula: C_{12}H_7Cl_3
Molecular Weight: 257.543
Melting Point (°C):
41  (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
247.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.694  (calculated-assuming ∆S_{fus} = 56 J/mol K, Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C):
0.402  (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.162  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.223  (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0402  (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0291  (GC-RI correlation, Burkhard et al. 1985b)
0.0447  (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)
log (P₁/Pa) = –4075/(T/K) + 12.36, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
25.74  (calculated-P/C, Burkhard et al. 1985a)
35.6  (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.26  (calculated-QSPR, Dunnivant et al. 1992)
29.0  (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –∆H_{fus}/RT + ∆S_{fus}/R; R is the ideal gas constant, ∆H_{fus} = 41 ± 4 kJ/mol, ∆S_{fus} = 0.10 ± 0.02 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
5.44  (calculated-TSA, Burkhard 1984)
5.53  (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.57  (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.6729  (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
8.17  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log $K_{OC}$:
5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14–30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9–15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.24 2,3,6-Trichlorobiphenyl (PCB-24)

Common Name: 2,3,6-Trichlorobiphenyl
Synonym: PCB-24, 2,3,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3,6-trichlorobiphenyl
CAS Registry No: 55702-45-9
Molecular Formula: C_{12}H_{7}Cl_{7}
Molecular Weight: 257.543
Melting Point (°C):
49 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.581 (mp at 49°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.507 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.132 (20°C, supercooled liquid, Murphy et al. 1987)
0.0677, 0.118, 0.0604, 0.098 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
0.514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.167; 0.136, 0.358 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.132; 0.853 (quoted exptl., calculated-mp and K_{OW} Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.087 (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0899 (GC-RI correlation, Burkhard et al. 1985b)
0.0166 (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.6 - 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0708 (supercooled liquid Pₗ, GC-RI correlation, Fischer et al. 1992)
log (Pₗ/Pa) = – 3935/(T/K) + 12.02 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
44.18 (calculated-P/C, Burkhard et al. 1985a)
32.12 (20°C, Murphy et al. 1987)
34.35 (calculated-molecular-connectivity indices, Sabljic & Güsten 1989)
22.3 (wetted-wall column-GC, Brunner et al. 1990)
31.53 (calculated-QSPR, Dunnivant et al. 1992)
32.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ∆H_{f}/RT + ∆S_{f}/R; R is the ideal gas constant, ∆H_{f} = 39 ± 21 kJ/mol, ∆S_{f} = 0.10 ± 0.07 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 4.52, 5.67 (RP-HPLC-$k'$ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 5.45, 5.42, 5.44, 5.46 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.44 (recommended, Sangster 1993)
- 5.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 7.75 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 5.16 (suspended particulate matter, Burkhard 1984)
- 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
- Photolysis: $k = (0.019–0.029) \text{ min}^{-1}$ with $t_\frac{1}{2} = 24–36 \text{ min}$, $k = (0.041–0.059) \text{ min}^{-1}$ with $t_\frac{1}{2} = 12–17 \text{ min}$ and $k = (0.12–0.22) \text{ min}^{-1}$ with $t_\frac{1}{2} = 3–6 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; rate constants, $k = (0.0066–0.030) \text{ min}^{-1}$ with $t_\frac{1}{2} = 23–105 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; rate constant $k = 0.022 \text{ min}^{-1}$ with $t_\frac{1}{2} = 31 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.7 – 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14–30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.6 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_\frac{1}{2} \sim 4–11 \text{ d}$ in freshwater systems, $t_\frac{1}{2} = 0.1–10 \text{ d}$ in cloud water, $t_\frac{1}{2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9–15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.008 \text{ d}^{-1}$ with $t_\frac{1}{2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.009 \text{ d}^{-1}$ with $t_\frac{1}{2} = 81 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime $\tau = 14–30 \text{ d}$ due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime $\tau = 6.9–17 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Polychlorinated Biphenyls (PCBs)

Surface water: half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991); $t_{1/2} = 24–36$ min, 12–17 min and 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO$_2$, respectively; $t_{1/2} = 23–105$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO$_2$; $t_{1/2} = 31$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO$_2$ (Huang et al. 1996).

Ground water:
Sediment:
Soil:
Biota: depuration t$_{1/2} = 91$ d for high-dose treatment, t$_{1/2} = 81$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.25 2,3′,4-Trichlorobiphenyl (PCB-25)

Common Name: 2,3′,4-Trichlorobiphenyl
Synonym: PCB-25, 2,3′,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,4-trichlorobiphenyl
CAS Registry No: 55712-37-3
Molecular Formula: C₁₂H₇Cl₃
Molecular Weight: 257.543
Melting Point (°C): 61 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH$_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, ΔS$_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS$_{\text{fus}}$ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.317 (supercooled liquid $S_L$, Burkhard et al. 1985a)
0.025 (supercooled liquid $S_L$, Murphy et al. 1987)
0.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.1025 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0313 (P$_L$, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0327 (GC-RI correlation, Burkhard et al. 1985b)
0.0373, 0.0366 (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.24 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
0.0295, 0.0372 (supercooled liquid P$_L$, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P$_L$/Pa) = −4075/(T/K) + 12.24 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
25.53 (calculated-P/C, Burkhard et al. 1985a)
43.27 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.04 (calculated-QSPR, Dunnivant et al. 1992)
17.20 (calculated-QSPR, Achman et al. 1993)
14.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K$_{\text{AW}}$ = −ΔH$_{\text{fus}}$/RT + ΔS$_{\text{fus}}$/R; R is the ideal gas constant, ΔH$_{\text{fus}}$ = 39 ± 21 kJ/mol, ΔS$_{\text{fus}}$ = 0.10 ± 0.07 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K$_{\text{ow}}$:
5.51 (calculated-TSA, Burkhard 1984)
5.67 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.54 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.63 (calculated, Miertus & Jakus 1990)
5.54 (recommended, Sangster 1993)
5.6793 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 9.31; 8.28; 8.23 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  $k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14$–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
  $k_{OH}(\text{aq.}) = 7.2 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{1/2} = 0.1$–10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
  $k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9$–5 d at room temp. (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

- Surface water: half-lives range from $t_{1/2} = 4$–11 d in freshwater systems, $t_{1/2} = 0.1$–10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 87$ d for high-dose treatment, $t_{1/2} = 102$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.26 2,3′,5-Trichlorobiphenyl (PCB-26)

Common Name: 2,3′,5-Trichlorobiphenyl
Synonym: PCB-26, 2,3′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,5-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: C$_{12}$H$_7$Cl$_3$
Molecular Weight: 257.543
Melting Point (°C): 40.0–40.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}}$ = 56 J/mol K), F: 0.705 (mp at 40.5°C)
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
0.219, 0.166, 0.205, 0.155 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.253 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.138 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0353 (supercooled liquid $P_L$, Burkhard et al. 1984)
0.0262 (GC-RI correlation, Burkhard et al. 1985a)
0.0363 (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
0.0411, 0.0412 (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0182 (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0316, 0.389 (supercooled liquid $P_L$, GC-RI correlation, different stationary phases Fischer et al. 1992)
log ($P_t/P_a$) = - 4075/(T/K) + 12.28 (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)
0.0112–0.0402; 0.0182–0.0449 (literature $P_s$ range; literature $P_L$ range, Delle Site 1997)
Henry’s Law Constant (Pa m$^3$/mol at 25°C):
32.93 (gas stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
20.27 (wetted-wall column-GC, Brunner et al. 1990)
12.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
30.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = - \Delta H_{f/R} + \Delta S_{f/R}$; R is the ideal gas constant, $\Delta H_{f} = 41 \pm 21$ kJ/mol, $\Delta S_{f} = 0.10 \pm 0.08$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{ow}$:
5.76 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.52, 5.68, 5.72, 5.68 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.65 (recommended, Sangster 1993)
5.76 (recommended, Hansch et al. 1995):
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 9.30, 8.27; 8.24 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
- 8.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:
- 5.31 (suspended particulate matter, Burkhard 1984)
- 6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}(calc) = (0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}(aq.) = 6.3 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}(calc) = (1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9–15$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_2 = 0.007$ d$^{-1}$ with $t_{\frac{1}{2}} = 105$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005$ d$^{-1}$ with $t_{\frac{1}{2}} = 135$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{\frac{1}{2}} \sim 4–11$ d in freshwater systems, $t_{\frac{1}{2}} = 0.1–10$ d in cloud water, $t_{\frac{1}{2}} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{\frac{1}{2}} = 105$ d for high-dose treatment, $t_{\frac{1}{2}} = 135$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.27 2,3′,6-Trichlorobiphenyl (PCB-27)

Common Name: 2,3′,6-Trichlorobiphenyl
Synonym: PCB-27, 2,3′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,6-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 257.543
Melting Point (°C): 45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 42 ± 6
Entropy of Fusion, ΔS_{fus} (J/mol K): 0.10 ± 0.02
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.404 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.039 (supercooled liquid S_L, Murphy et al. 1987)
0.256 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0653 (P_L, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0676 (GC-RI correlation, Burkhard et al. 1985b)
0.0598, 0.0628 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.26 × 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0490, 0.0708 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3935/(T/K) + 11.97 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard et al. 1985a)
49.95 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
41.0 (calculated-QSPR, Dunnivant et al. 1992)
22.17 (quoted as PCB-24 and 27, Achman et al. 1993)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ΔH_{f} / RT + ΔS_{f} / R; R is the ideal gas constant, ΔH_{f} = 42 ± 6 kJ/mol, ΔS_{f} = 0.10 ± 0.02 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
5.43 (calculated-TSA, Burkhard 1984)
5.44 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.52 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.50 (quoted as PCB-24 and 27, Murray & Andren 1992)
5.2417 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
7.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 5.23 (suspended particulate matter, Burkhard 1984)
- 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(aq.) = 7.6 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $\sim$4–11 d in freshwater systems, 0.1–10 d in cloud water, $>1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
  - $k_{OH}(calc) = (1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9–15$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.008$ d$^{-1}$ with $t_\frac{1}{2} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.009$ d$^{-1}$ with $t_\frac{1}{2} = 81$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_\frac{1}{2} \sim 4–11$ d in freshwater systems, $t_\frac{1}{2} = 0.1–10$ d in cloud water, $t_\frac{1}{2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration $t_\frac{1}{2} = 91$ d for high-dose treatment, $t_\frac{1}{2} = 81$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.28 2,4,4′-Trichlorobiphenyl (PCB-28)

![Chemical Structure](image)

Common Name: 2,4,4′-Trichlorobiphenyl
Synonym: PCB-28, 2,4,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,4,4′-trichlorobiphenyl
CAS Registry No: 7012-37-5
Molecular Formula: C_{12}H_{7}Cl_{3}
Molecular Weight: 257.543
Melting Point (°C):
57–58  (Hutzinger et al. 1971, 1974)
Boiling Point (°C):
206–207  (Sengupta 1966)
Density (g/cm³ at 20°C): 1.1485
Molar Volume (cm³/mol):
247.3  (calculated-Le Bas method at normal boiling point)
198.7  (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
56.6  (Passivirta et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$:
0.482  (Mackay et al. 1980; Shiu & Mackay 1986)
0.482  (Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.085  (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.260  (generator column-GC/ECD, Weil et al. 1974)
0.119  (Dexter & Pavlou 1978)
0.270  (20°C, supercooled liquid $S_L$, shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985)
0.142  (generator column-HPLC/UV, Huang 1983)
0.163  (generator column-GC/ECD, Miller et al. 1984)
0.312  (supercooled liquid $P_L$, calculated-TSA, Burkhard et al. 1985b)
0.116  (shake flask-GC/ECD, Chiou et al. 1986)
0.143  (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixture, Murphy et al. 1987)
0.177, 0.107, 0.144, 0.117  (RP-HPLC-k correlation, different stationary and mobile Brodsky & Ballschmiter 1988)
0.067  (22°C, generator column-GC, Opperhuizen et al. 1988)
0.117  (generator column-GC, Dunnivant & Elzerman 1988)
$\log \left[ S_L/(\text{mol/L}) \right] = 0.232 - 975.5/(T/K)$; (supercooled liquid, Passivirta et al. 1999)
0.260, 0.228  (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log \left[ S_L/(\text{mol m}^{-3}) \right] = -1147/(T/K) + 0.79$ (supercooled liquid, final adjusted eq., Li et al. 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0277  (supercooled liquid $P_L$, Burkhard 1984)
0.014  (GC-RI correlation, Burkhard et al. 1985a)
0.0277  (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
0.0339, 0.0340  (supercooled $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0149  (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0277, 0.0335  (supercooled liquid, Dunnivant & Elzerman 1988)
$\log (P/\text{mmHg}) = 10.40 - 4270/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
Polychlorinated Biphenyls (PCBs)

0.257, 0.0324 (supercooled liquid \( P_L \); GC-RI correlation, different stationary phases, Fischer et al. 1992)
\[
\log (P_L/P_a) = -4075/(T/K) + 12.20 \quad \text{(supercooled liquid \( P_L \), GC-RT correlation, Falconer & Bidleman 1994)}
\]
0.0210; 0.0436 (solid, supercooled liquid, Passivirta et al. 1999)
\[
\log (P_L/P_a) = 15.15 - 5049/(T/K) \quad \text{(solid, Passivirta et al. 1999)}
\]
\[
\log (P_L/P_a) = 12.20 - 4075/(T/K) \quad \text{(supercooled liquid, Passivirta et al. 1999)}
\]
0.0234, 0.0436 (solid, supercooled liquid, Passivirta et al. 1999)
\[
\log (P_S/P_a) = 15.15 - 5049/(T/K) \quad \text{(solid, Passivirta et al. 1999)}
\]
\[
\log (P_L/P_a) = 12.20 - 4075/(T/K) \quad \text{(supercooled liquid, Passivirta et al. 1999)}
\]
0.0234, 0.0436 (supercooled liquid \( P_L \); LDV literature derived value, FA V final adjusted value, Li et al. 2003)
\[
\log (P_L/P_a) = -4157/(T/K) + 12.31 \quad \text{(supercooled liquid, linear regression of literature data, Li et al. 2003)}
\]
\[
\log (P_L/P_a) = -4007/(T/K) + 11.87 \quad \text{(supercooled liquid, final adjusted eq., Li et al. 2003)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations

32.02 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.7, 21.2, 47.4, 50.3, 70.8, 120.6, 122.2 (10.4, 20, 30.1, 34.9, 42.1, 47.9, 48.4°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
\[
\log \left[ H/(Pa \cdot m^3/mol) \right] = 11.97 - 3100/(T/K); \quad \text{(Passivirta et al. 1999)}
\]
13.13, 19.06, 27.18, 38.14 ± 0.37, 50.39 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
\[
K_{AW} = \exp \left[ - \frac{(32.5/kJ \cdot mol^{-1})}{RT} + \frac{(0.074/kJ \cdot mol^{-1} \cdot K^{-1})}{R} \right]; \quad \text{where } R = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \text{ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)}
\]
19.72 (20°C, selected from reported experimentally measured values, Staedinger & Roberts 1996, 2001)
\[
\log K_{AW} = 6.324 - 2467/(T/K) \quad \text{(van’t Hoff eq. derived from literature data, Staedinger & Roberts 2001)}
\]
36.5 (exptl. data, Bamford et al. 2002)
\[
\ln K_{AW} = - \frac{\Delta H_{H}/RT + \Delta S_{H}/R; \quad R \text{ is the ideal gas constant, } \Delta H_{H} = 33 \pm 2 \text{ kJ/mol, } \Delta S_{H} = 0.07 \pm 0.01 \text{ kJ/mol} \cdot \text{K}}{(Bamford et al. 2002)—see Comment by Goss et al. 2004}
\]
33.11, 30.2 (LDV literature-derived value, FA V final adjusted value, Li et al. 2003)
\[
\log \left[ H/(Pa \cdot m^3/mol) \right] = -2010/(T/K) + 857 \quad \text{(LDV linear regression of literature data, Li et al. 2003)}
\]
\[
\log \left[ H/(Pa \cdot m^3/mol) \right] = -2860/(T/K) + 11.08 \quad \text{(FA V final adjusted eq., Li et al. 2003)}
\]

Octanol/Water Partition Coefficient, log \( K_{OW} \):

4.38 (shake flask-GC, Paris et al. 1978)
5.74 (RP-TLC-k’ correlation, Bruggeman et al. 1982)
5.62 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.51, 5.77, 5.81, 5.74 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.68 (generator column-GC, Larsen et al. 1992)
5.59 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
5.71 (recommended, Sangster 1993)
5.62 (recommended, Hansch et al. 1995)
5.55, 5.66 (LDV literature-derived value, FA V final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated and reported temperature dependence equations:

7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
\[
\log K_{OA} = -6.12 + 4190/(T/K) \quad \text{(fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)}
\]
8.76 (10°C, estimated, Thomas et al. 1997)
9.43, 8.40 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
\[
7.93, 7.85 \quad \text{(LDV literature derived value, FA V final adjusted value, Li et al. 2003)}
\]
\[
\log K_{OA} = 4102/(T/K) - 5.91 \quad \text{(FA V final adjusted eq., Li et al. 2003)}
\]

Bioconcentration Factor, log \( BCF \):

2.60–3.82 (various marine species, mean dry wt. BCF, Hope et al. 1998)
3.82–4.93 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.32, 5.62 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.74, 5.66 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$

- 5.50, 4.70 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log $K_{OM}$ at 25°C or as indicated:

- 4.23 (calculated, Kenaga 1980)
- 4.38 (log $K_{OM}$ soil organic matter, Wood burn soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
- 5.31 (suspended particulate matter, Burkhard 1984)
- 5.28 (sediment: suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
- 5.30; 4.59 (suspended solids-Lake Superior: calculated-$K_{OM}$, Baker et al. 1986)
- 4.40; 3.54 (Sanhedron soil-Suwannee River; humic acid, shake flask-GC, Chiou et al. 1986, 1987)
- 5.31 (suspended particulate matter, Baker et al. 1984)
- 5.28 (sediment: suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
- 4.84; 4.24 (Fluka-Tridom humic acid; Calcasieu River humic extract, Chiou et al. 1987)
- 5.33; 3.27 (Suwannee River water sample; Sopchoppy River water sample, Chiou et al. 1987)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.03–4.91; 5.30–5.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.25; 5.27, 4.91, 5.32 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

**Vaporization:**

- Photolysis: photolysis rate $k_p$ (exptl) = $6 \times 10^{-8}$ d$^{-1}$ with $t_{1/2} = 133$ d; $k_p$ (calc) = $2.2 \times 10^{-8}$ d$^{-1}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}$ (calc) = $(0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$ (calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}$ (aq) = $7.2 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from 4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
  - $k_{OH}$ (calc) = $(1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau$ (calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

**Hydrolysis:**

- Biodegradation: $t_{1/2} = 7$ h of biodegradation by Alcaligenes sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980); 49% degradation at 72 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism Alcaligenes eutrophus H850 (Bedard et al. 1986).

**Biotransformation:**

- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 0.016$ d$^{-1}$ with $t_{1/2} = 44$ d and $k_2 = 0.015$ d$^{-1}$ with $t_{1/2} = 46$ d for food concn of 16 ng/g and 108 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
  - $k_1 = 0.00054$ h$^{-1}$; $k_2 = 0.089$ h$^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
  - $k_2$ (calc) = 11 (food lipid (mg)/(g worm lipid-d)); $k_2$ (calc) = 0.14 d$^{-1}$ (earthworm, Wågman et al. 2001)
  - $k_2$ = 0.008 d$^{-1}$ with $t_{1/2} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_2$ = 0.008 d$^{-1}$ with $t_{1/2} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995);

t_{1/2} = 72 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis t_{1/2} = 133 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);

half-lives range from t_{1/2} ~ 4–11 d in freshwater systems, t_{1/2} = 0.1–10 d in cloud water, t_{1/2} > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

t_{1/2} = 1450 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: t_{1/2} = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.15 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 1.34 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.53 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00378 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00183 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.0016 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00044 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

t_{1/2} = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: depuration t_{1/2} = 44–46 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

t_{1/2} = 7.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination t_{1/2} = 5 d in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration t_{1/2} = 91 d for high-dose treatment, t_{1/2} = 88 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.29 2,4,5-Trichlorobiphenyl (PCB-29)

Common Name: 2,4,5-Trichlorobiphenyl
Synonym: PCB-29, 2,4,5-trichloro-1,1′-biphenyl
Chemical Name: 2,4,5-trichlorobiphenyl
CAS Registry No: 15862-07-4
Molecular Formula: C_{12}H_{7}Cl_{3}
Molecular Weight: 257.543
Melting Point (°C): 78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.1485
Molar Volume (cm³/mol):
   247.3 (calculated-Le Bas method at normal boiling point)
   198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
   22.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ∆S_{fus} (J/mol K):
   65.27 (Miller et al. 1984)
   65.24, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
   0.30 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   0.092 (generator column-GC/ECD, Weil et al. 1974)
   0.119 (Dexter & Pavlou 1978)
   0.140 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
   0.142 (generator column-HPLC/UV, Huang 1983)
   0.162 (generator column-GC/ECD, Miller et al. 1984, 1985)
   0.0.098, 0.107,0.138,0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
   0.106* ± 0.0045 (generator column-GC/ECD, Shiu et al. 1997)
   0.0413, 0.0682, 0.106, 0.203, 0.33 (5, 15, 25, 35, 45°C, generator column-GC, Shiu et al. 1997)
   ln x = −3.06175 − 4633.86/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
   0.479, 0.389 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
   log S/L/(mol m⁻³) = −824/(T/K) + 0.03 (supercooled liquid, linear regression of literature data, Li et al. 2003)
   log S/L/(mol m⁻³) = −977/(T/K) + 0.46 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   0.0443 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
   0.0112 (GC-R1 correlation, Burkhard et al. 1985a)
   0.0320 (supercooled liquid P_L, GC-R1 correlation, Burkhard et al. 1985b)
   0.0453, 0.0464 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
   log (P_L/Pa) = −4075/(T/K) + 12.20 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
   0.0263 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
   0.0447, 0.0457 (supercooled liquid P_L; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
   log P_L/Pa = −3904/(T/K) + 11.75 (supercooled liquid, final adjusted eq., Li et al. 2003)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section):

20.27 (wetted-wall column-GC; Brunner et al. 1990; quoted, Achman et al. 1993)
37.89* ± 0.53 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)

\[ \ln K_{AW} = 9.863 - 4197.74/(T/K); \text{ temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)} \]

\[ K_{AW} = \exp \left\{ \left( -\frac{34.9}{\text{kJ·mol}^{-1}} \right)/R \right\} \text{ temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)} \]

36.3 (exptl. data, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_f/RT + \Delta S_f/R; \text{ R is the ideal gas constant, } \Delta H_f = 35 \pm 3 \text{ kJ/mol, } \Delta S_f = 0.08 \pm 0.01 \text{ kJ/mol·K} \]
(Bamford et al. 2002)—see Comment by Goss et al. 2004

32.36, 30.20 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

\[ \log \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] = -1674/(T/K) + 7.13 \text{ (LDV linear regression of literature data, Li et al. 2003)} \]

\[ \log \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] = -2927/(T/K) + 11.30 \text{ (FAV final adjusted eq., Li et al. 2003)} \]

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations:

6.22 (Hansch & Leo 1979)

5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)

5.86 (HPLC-RT correlation, Woodburn 1982)

5.51 (generator column-GC/ECD, Miller et al. 1984)

5.81 (generator column-GC, Woodburn et al. 1984)

5.86 (HPLC-RT correlation, Woodburn et al. 1984)

6.25 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.66 (HPLC-RP/MS, Burkhard & Kuehl 1986)

5.81 (generator column-GC/ECD, Doucette & Andren 1987)

5.78, 5.82, 5.88, 5.76 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.86 (shake flask/slow stirring-GC, De Bruijn et al. 1989)

5.901 ± 0.007 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)

5.54 (HPLC-k′ correlation, Noegrohati & Hammers 1992)

5.81 (recommended, Sangster 1993)

5.90 (recommended, Hansch et al. 1995)

5.74, 5.60 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section:

7.96* (generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)

\[ \log K_{OA} = -4.80 + 3791.7/(T/K); \text{ temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)} \]

8.03 (20°C, generator column-GC, Harner & Bidleman 1996)

\[ \log K_{OA} = -4.77 + 3792/(T/K); \text{ temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)} \]

9.15, 8.05 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)

8.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

8.01; 8.03 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

8.80, 7.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

\[ \log K_{OA} = 4175/(T/K) - 6.22 \text{ (FAV final adjusted eq., Li et al. 2003)} \]

Bioconcentration Factor, log BCF:

4.97 (guppy, lipid wt. based, Gobas et al. 1989)

5.41 (guppy, corr. lipid wt. based, Gobas et al. 1989)

4.36, 5.53 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.26 (suspended particulate matter, Burkhard 1984)

4.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

© 2006 by Taylor & Francis Group, LLC
Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

**Volutilization:**
rate constants \( k = (0.019–0.022) \text{ min}^{-1} \) with \( t_{1/2} = 31–36 \text{ min} \), \( k = (0.033–0.048) \text{ min}^{-1} \) with \( t_{1/2} = 14–21 \text{ min} \) and \( k = (0.13–0.14) \text{ min}^{-1} \) with \( t_{1/2} = 5 \text{ min} \) in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UV A-340 in the presence of 25, 50 and 100 \( \mu \text{g/mL} \) TiO\(_2\), respectively; rate constants \( k = (0.0056–0.020) \text{ min}^{-1} \) with \( t_{1/2} = 35–123 \text{ min} \) in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 \( \mu \text{g/mL} \) TiO\(_2\) (Huang et al. 1996).

**Photolysis:**
rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:

\[ k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 14–30 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)} \]

\[ k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 6.9–15 \text{ d at room temp. (Kwok et al. 1995)} \]

**Oxidation:**
rate constant \( k \), with NO\(_3\) radical and \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:

Hydrolysis:

**Biodegradation:**
half-life of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments estimated to be less than 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

**Biotransformation:**

**Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:**

<table>
<thead>
<tr>
<th>Condition</th>
<th>( k_2 ) Value</th>
<th>( t_{1/2} ) Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fish, quoted, Hawker &amp; Connell 1985; Thomann 1989</td>
<td>( 0.004 \text{ d}^{-1} )</td>
<td>( 190 \text{ d} ) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt. high-dose treatment, Buckman et al. 2004)</td>
</tr>
<tr>
<td>8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt. high-dose + CYPIA-inducing compounds (hCYP) treatment</td>
<td>( 0.007 \text{ d}^{-1} )</td>
<td>( 100 \text{ d} ) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt. high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)</td>
</tr>
</tbody>
</table>

Half-Lives in the Environment:

**Air:**
calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

**Surface water:**
\( t_{1/2} = 31–36 \text{ min} \), 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 \( \mu \text{g/mL} \) TiO\(_2\), respectively; \( t_{1/2} = 35–123 \text{ min} \) in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 \( \mu \text{g/mL} \) TiO\(_2\) (Huang et al. 1996).

**Groundwater:**

**Sediment:**

**Soil:**

**Biota:**

depuration \( t_{1/2} = 190 \text{ d} \) for high-dose treatment, \( t_{1/2} = 100 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
TABLE 7.1.1.29.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficient log of 2,4,5-trichlorobiphenyl (PCB-29) at various temperatures

<table>
<thead>
<tr>
<th>Solubility</th>
<th>Henry's law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-GC/ECD</td>
<td>t/°C</td>
<td>S/g·m$^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>0.0413</td>
</tr>
<tr>
<td>15</td>
<td>11</td>
<td>0.0682</td>
</tr>
<tr>
<td>25</td>
<td>18</td>
<td>0.106</td>
</tr>
<tr>
<td>35</td>
<td>25</td>
<td>0.203</td>
</tr>
<tr>
<td>45</td>
<td>31</td>
<td>0.330</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = 36.9 \]

at 5–45°C

\[ \ln K_{\text{AW}} = -\frac{\Delta H}{R} + \frac{\Delta S}{R} \]

\[ K_{\text{AW}} = A + B/T \]

\[ \Delta H_{\text{OA}}/(kJ \text{ mol}^{-1}) = 72.6 \]

\[ \Delta S/(J \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) = 82 \pm 10 \]

FIGURE 7.1.1.29.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,4,5-trichlorobiphenyl (PCB-29).
7.1.1.30 2,4,6-Trichlorobiphenyl (PCB-30)

Common Name: 2,4,6-Trichlorobiphenyl
Synonym: PCB-30
Chemical Name: 2,4,6-trichlorobiphenyl
CAS Registry No: 35693-92-6
Molecular Formula: C$_{12}$H$_7$Cl$_3$
Molecular Weight: 257.543
Melting Point (°C): 62.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
- 247.3 (calculated-Le Bas method at normal boiling)
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):
- 16.5 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999))
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):
- 49.37 (Miller et al. 1984)
- 49.36, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), $F$:
- 0.427 (Shiu & Mackay 1986)

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.226 (generator column/ECD, Miller et al. 1984, 1985)
- 0.024, 0.0468, 0.0491, 0.0893 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmieder 1988)
- 0.187* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
- 0.0803, 0.187, 0.435 (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
- S/(mol/L) = 2.49 × 10$^{-7}$ exp(0.047·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
- log $x$ = – 1742/(T/K) − 1.983, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
- 0.252, 0.243 (generator column-GC, Dunnivant & Elzerman 1988)
- 0.236 (generator column-GC, Li et al. 1992)
- 0.235 (generator column-GC/ECD, Li et al. 1993)
- 0.217 (shake flask-GC/ECD, Li & Andren 1994)
- ln $x$ = – 4.5969 – 4004.7/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.031 (Augood 1953; quoted, Bidleman 1984)
- 0.0865, 0.0948(P$_{\text{GC}}$ by GC-RT correlation, different stationary phases, Bidleman 1984)
- 0.030 (supercooled liquid $P_L$, converted from literature $P_S$ with $\Delta S_{\text{ fus}}$ Bidleman 1984)
- 0.0955, 0.144 (supercooled liquid $P_L$ calculated from $P_{\text{GC}}$, GC-RT correlation, different stationary phases, Bidleman 1984)
- 0.0421 (GC-RI correlation, Burkhard et al. 1985a)
- 0.111, 0.135 (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.0946 (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
- 0.110; 0.0851 (supercooled liquid $P_L$; GC-RI correlation, different stationary phases, Fischer et al. 1992)
- log ($P_S$/Pa) = – 3886/(T/K) + 12.02; (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)
- 0.0130–0.0637; 0.085–0.146 (literature $P_S$ range; literature $P_L$ range, Delle Site 1997)
Henry’s Law Constant (Pa m³/mol at 25°C):

61.40 (calculated-P/C, Burkhard et al. 1985b)
49.51 (calculated-P/C, Shiu & Mackay 1986)
65.76 (batch stripping, Dunnivant et al. 1988 Dunnivant & Elzerman 1988)
47.51 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
58.04 (calculated-QSPR, Dunnivant et al. 1992)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H/R + \Delta S/R; R \text{ is the ideal gas constant, } \Delta H = 42 \pm 6 \text{ kJ/mol, } \Delta S = 0.10 \pm 0.01 \text{ kJ/mol-K} \]

Octanol/Water Partition Coefficient, log \( K_{OW} \):

5.47 (generator column-GC/ECD, Miller et al. 1984, 1985)
5.57 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
5.77, 5.70, 5.51, 5.48 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
5.33, 5.57 (RP-HPLC-k′ correlation, different stationary phases, Sherblom & Eganhouse 1988)
5.71 ± 0.014 (shake flask/slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.75 (generator column-GC, Li et al. 1993)
5.62 (recommended, Sangster 1993)
5.71 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

7.28 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

5.24 (suspended particulates matter, Burkhard 1984)
4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
with NO_{3} radical and k_{O3} with O_{3} or as indicated, *data at other temperatures see reference:

\[ k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 14–30 \text{ d, due to gas-phase loss process at room temp.} \]

\[ k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 6.9–15 \text{ d at room temp.} \]

Hydrolysis:

Biodegradation: 30% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism \textit{Alcaligenes eutrophus} H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:
### 7.1.1.31 2,4′,5-Trichlorobiphenyl (PCB-31)

![Chemical Structure](image_url)

**Common Name:** 2,4′,5-Trichlorobiphenyl  
**Synonym:** PCB-31, 2,4′,5-trichloro-1,1′-biphenyl  
**Chemical Name:** 2,4′,5-trichlorobiphenyl  
**CAS Registry No:** 16606-02-3  
**Molecular Formula:** C\(_{12}\)H\(_7\)Cl\(_3\)  
**Molecular Weight:** 257.543

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>67 (Bellavita 1935; Hutzinger et al. 1974)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm(^3))</td>
<td></td>
</tr>
</tbody>
</table>
| Molar Volume (cm\(^3\)/mol)     | 247.3 (calculated-Le Bas method at normal boiling point)  
|                                 | 198.7 (Ruelle & Kesselring 1997)            |
| Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol) |                                     |
| Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K) |                                      |
| Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), F | 0.384 (Shiu & Mackay 1986) |
| Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations): |                                      |
|                                 | 0.11 (Kilzer et al. 1979)                  |
|                                 | 0.075 (shake flask-GC/ECD, Bruggeman et al. 1981) |
|                                 | 0.265, 0.155, 0.179, 0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988) |
|                                 | 0.090 (generator column-GC/ECD, Opperhuizen et al. 1988) |
|                                 | 0.143 (20°C, supercooled liquid S\(_L\), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987) |
|                                 | 0.220, 0.194 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003) |
|                                 | log S\(_L\)/(mol m\(^3\)) = −1123/(T/K) + 0.64 (supercooled liquid, final adjusted eq., Li et al. 2003) |
| Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations): |                                      |
|                                 | 0.0341, 0.0474 (supercooled liquid P\(_L\), GC-RT correlation, different stationary phases, Bidleman 1984) |
|                                 | 0.0132 (GC-RI correlation, Burkhard et al. 1985a) |
|                                 | 0.0313 (supercooled liquid P\(_L\), calculated-GC-RI correlation, Burkhard et al. 1985b) |
|                                 | 0.0373, 0.0346 (supercooled liquid P\(_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985) |
|                                 | 0.0149 (20°C, supercooled liquid P\(_L\), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987) |
|                                 | log (P/Pa) = 10.40 – 4270/(T/K) (GC-RT correlation, Tateya et al. 1988) |
|                                 | 0.0263, 0.0347 (supercooled liquid P\(_L\), GC-RI correlation, different stationary phases, Fischer et al. 1992) |
|                                 | 0.024, 0.0257 (supercooled liquid P\(_L\), LDV literature derived value, FAV final adjusted value, Li et al. 2003) |
|                                 | log (P\(_L\)/Pa) = −4149/(T/K) + 12.29 (supercooled liquid, linear regression of literature data, Li et al. 2003) |
|                                 | log (P\(_L\)/Pa) = −4010/(T/K) + 11.86 (supercooled liquid, final adjusted eq., Li et al. 2003) |

**Henry’s Law Constant (Pa m\(^3\)/mol at 25°C or as indicated and reported temperature dependence equations):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>94.13</td>
<td>(gas-stripping-GC, Atlas et al. 1982)</td>
</tr>
<tr>
<td>20.26</td>
<td>(calculated, Murphy et al. 1983)</td>
</tr>
<tr>
<td>25.43</td>
<td>(calculated-P/C, Burkhard et al. 1985b)</td>
</tr>
<tr>
<td>26.75</td>
<td>(20°C, calculated-P/C, Murphy et al. 1987)</td>
</tr>
</tbody>
</table>
Polychlorinated Biphenyls (PCBs)

28.47 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
27.78 (calculated-QSPR, Dumnivant et al. 1992)
20.21 (calculated-QSPR, Achman et al. 1993)
12.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
30.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_i^R/RT + \Delta S_i^R/R$; R is the ideal gas constant, $\Delta H_i$ = 41 ± 21 kJ/mol, $\Delta S_i$ = 0.10 ± 0.08 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
37.15, 33.88 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa m^3/mol)] = -2887/(T/K) + 11.22$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
6.22 (Hansch & Leo 1979)
5.30 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
5.77 (RP-TLC-‘k’ correlation, Bruggeman et al. 1982)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.79 (generator column-GC/ECD, Woodburn et al. 1984)
5.70 (selected, Shiu & Mackay 1986)
5.99, 6.22, 6.18, 6.33 (RP-HPLC-‘k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
5.59 (HPLC-‘k’ correlation, Noegrohati & Hammers 1992)
5.68 (recommended, Sangster 1993)
5.79 (recommended, Hansch et al. 1995)
5.79, 5.78 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:
7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = -6.12 + 4190/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.43, 8.40; 8.23 (0, 20°C, multi-column GC-‘k’ correlation; calculated at 20°C, Zhang et al. 1999)
8.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.93, 7.94 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4110/(T/K) - 5.84$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:
3.45 (fish, Korte et al. 1978)
–0.30, –0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
5.98 (goldfish, 10% lipid content in food, Bruggeman et al. 1981)
3.95, 3.95, 4.51 (algae, fish, activated sludge, Freitag et al. 1984, 1985)
3.66 (salmon fry in humic water-steady state, Carlberg et al. 1986)
3.83 (salmon fry in lake water-steady state, Carlberg et al. 1986)
4.62 (fish, calculated-C_p/C_w or k_v/k_2 Connell & Hawker 1988; Hawker 1990)
4.66; 6.19 (zebrafish: log $BCF_p$ wet wt basis; log $BCF_l$ lipid wt basis, Fox et al. 1994)
4/09 (algae $Chlorella fusca$, wet wt basis, Wang et al. 1996)
5.04 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
3.95, 4.65 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
4.23, 5.23 ($Daphna$: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.08, 6.04 (mussel: wet wt basis, dry wt basis, Geyer et al. 2000)
4.63, 5.93 (goldfish: wet wt basis, dry wt basis, Geyer et al. 2000)
4.67, 6.19 (zebrafish: wet wt basis, dry wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$
5.90, 4.80 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)
Sorption Partition Coefficient, $\log K_{OC}$:
- 5.31 (suspended particulates, Burkhard 1984)
- 5.5–6.3, 5.9; 6.80 (suspended sediment, average; algae > 50 $\mu$m, Oliver 1987a)
- 5.48 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 4.63 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.51 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioglu 1996)
- 5.10 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(aq.) = 7.2 \times 10^{9}$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}(calc) = (1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9–15$ d at room temp. (Kwok et al. 1995)
- Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 890$ d$^{-1}$; $k_2 = 0.021$ d$^{-1}$ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986)
  - $k_1 = 0.0035$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
  - $k_1 = 37.1$ h$^{-1}$; $k_2 = 1.142$ h (goldfish, quoted, Hawker & Connell 1985)
  - $k_1 = 2.95$ d$^{-1}$; $k_2 = 1.68$ d (fish, quoted, Connell & Hawker 1988; Thomann 1989)
  - $k_1 = 3950$ d$^{-1}$; $k_2 = 0.0867$ d$^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)
  - $k_1 = 5044$ h$^{-1}$; $k_2 = 0.411$ h$^{-1}$ (algae *Chlorella fusca*, Wang et al. 1996)
  - $k_1 = 0.0047$ h$^{-1}$; $k_2 = 0.100$ h$^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
  - $k_1 = 14$ L d$^{-1}$ g$^{-1}$ dry wt.; $k_2 = 0.129$ d$^{-1}$ (Baltic Sea blue mussels, flow-through exp. Gustafsson et al. 1999)
  - $k_1 = 0.008$ d$^{-1}$ with $t_{1/2} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp. high-dose treatment, Buckman et al. 2004)
  - $k_1 = 0.008$ d$^{-1}$ with $t_{1/2} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp. high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
- Surface water: half-lives range from, $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:
- Sediment:
Soil:
Biota: $t_{1/2} = 196$ d in rainbow trout, and $t_{1/2} = 81$ d in its muscle, (Niimi & Oliver 1983);
    $t_{1/2} = 30$ d in worms at $8^\circ$C (Oliver 1987c);
theoretical half-life to reach 90% steady-state tissue concn 5.4 d (Baltic Sea blue mussels, flow-
    through expt., Gustafsson et al. 1999);
    $t_{1/2} = 6.9$ h in blood plasma (ring doves, Drouillard & Norstrom 2000).
    depuration $t_{1/2} = 91$ d for high-dose treatment, $t_{1/2} = 88$ d for high-dose + enzyme CYPIA-inducing
    compounds (hCYP) treatment ($8^\circ$C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.32 2,4',6-Trichlorobiphenyl (PCB-32)

Common Name: 2,4',6-Trichlorobiphenyl
Synonym: PCB-32, 2,4',6-trichloro-1,1'-biphenyl
Chemical Name: 2,4',6-trichlorobiphenyl
CAS Registry No: 38444-77-8
Molecular Formula: C₁₂H₃Cl₇
Molecular Weight: 257.543
Melting Point (°C):
70 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHᵢₚ (kJ/mol):
Entropy of Fusion, ΔSᵢₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSᵢₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.399 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.355, 0.182, 0.129, 0.0778 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0578 (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.060 (GC-RI correlation, Burkhard et al. 1985b)
0.0543, 0.0562 (supercooled Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 16.10 – 4100/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0427, 0.0589 (supercooled liquid Pₗ; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P₁/Pₐ) = –3935/(T/K) + 11.93 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
37.29 (calculated-P/C, Burkhard 1984)
41.75 (calculated-QSAR-MCI χ, Sabljc & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
39.69 (calculated-QSPR, Dunnivant et al. 1990)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln Kᵦₛₜₜ = −ΔHᵢₚ/RT + ΔSᵢₚ/R; R is the ideal gas constant, ΔHᵢₚ = 42 ± 6 kJ/mol, ΔSᵢₚ = 0.10 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₒₜₜ:
4.60, 5.75 (RP-HPLC-k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.80 (selected, Shiu & Mackay 1986)
4.95, 5.29, 5.21, 5.52 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.47 (generator column-GC, Larsen et al. 1992)
5.49 (recommended, Sangster 1993)
5.75 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 7.72 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.50 + 4240/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
- 8.89, 7.97; 7.92 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al 1999)
- 7.49 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_{B}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase reaction with OH radical, $k_{OH}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}^{(calc)} = (0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau^{(calc)} = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}^{(aq.)} = 8.0 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
  - $k_{OH}^{(calc)} = (1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau^{(calc)} = 6.9–15$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_2 = 0.008$ d$^{-1}$ with $t_{1/2} = 85$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.006$ d$^{-1}$ with $t_{1/2} = 111$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
- Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 85$ d for high-dose treatment, $t_{1/2} = 111$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.33 2,3',4'-Trichlorobiphenyl (PCB-33)

Common Name: 2,3',4'-Trichlorobiphenyl
Synonym: PCB-33, 2,3',4'-trichlorobiphenyl, 2',3,4-trichloro-1,1'-biphenyl
Chemical Name: 2,3',4'-trichlorobiphenyl
CAS Registry No: 38444-86-9
Molecular Formula: C_{12}H_{7}Cl_{3}
Molecular Weight: 257.543
Melting Point (°C): 60–60.5 (Wallnöfer et al. 1973)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.1485
Molar Volume (cm³/mol):
   247.3 (calculated-Le Bas method at normal boiling point)
   198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
   0.452 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.078 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.291 (calculated-TSA, Mackay et al. 1980)
0.0796 (quoted lit. average, Yalkowsky et al. 1983)
0.371 (supercooled liquid S, calculated-TSA, Burkhard et al. 1985b)
0.246, 0.170, 0.103, 0.142 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.133 (20°C, supercooled liquid P, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.103 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
0.152 (calculated-QSPR, Dunnivant et al. 1992)
0.209 (calculated-group contribution, Kühne et al. 1995)
0.0833, 0.219 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.576 (calculated–mp and K_{ow}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0107 (P_{s} from GC-RT correlation, Westcott & Bidleman 1981)
0.0133, 0.0160 (solid P_{s}, 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
log (P_{s}/mmHg) = 1.09 – 1510/(T/K), temp range 30–40°C (gas saturation-GC/ECD, Westcott et al. 1981)
0.030 (P_{l} calculated from P_{s} using fugacity ratio F, Westcott et al. 1981)
0.0115 (GC-RI correlation, Burkhard et al. 1985a)
0.0243 (supercooled liquid P, GC-RI correlation, Burkhard et al. 1985b)
0.0264, 0.0219 (supercooled liquid P, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0136, 0.030 (selected P_{s}, P_{l}, Shiu & Mackay 1986)
0.0119 (20°C, supercooled liquid P, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P_{l}/mmHg) = 10.40 – 4330/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0137; 0.0272 (quoted; calculated-UNIFAC, Banerjee et al. 1990)
0.0214, 0.0295 (supercooled liquid P, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log \( (P_e/P_a) = -4075/(T/K) + 12.09 \) (supercooled liquid \( P_L \), GC-RT correlation, Falconer & Bidleman 1994)
0.00484–0.0270; 0.0119–0.030 (quoted lit. \( P_S \) range; lit. \( P_L \) range, Delle Site 1997)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C or as indicated):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.20</td>
<td>(calculated, Murphy et al. 1983)</td>
</tr>
<tr>
<td>16.92</td>
<td>(calculated-P/C, Burkhard et al. 1985b)</td>
</tr>
<tr>
<td>43.67</td>
<td>(calculated-P/C, Shiu &amp; Mackay 1986)</td>
</tr>
<tr>
<td>22.70</td>
<td>(20°C, calculated-P/C, Murphy et al. 1987)</td>
</tr>
<tr>
<td>21.99</td>
<td>(calculated-QSAR-MCI ( \chi ), Sabljic &amp; Güsten 1989)</td>
</tr>
<tr>
<td>16.21</td>
<td>(wetted wall column-GC/ECD, Brunner et al. 1990)</td>
</tr>
<tr>
<td>24.31</td>
<td>(calculated-QSPR, Dunnivant et al. 1992)</td>
</tr>
<tr>
<td>11.9</td>
<td>(11°C, gas stripping-GC/ECD, Bamford et al. 2002)</td>
</tr>
<tr>
<td>29.2</td>
<td>(from 11°C exptl. data and compensation point, Bamford et al. 2002)</td>
</tr>
</tbody>
</table>

\[ \ln K_{AW} = -\frac{\Delta H_H}{RT} + \frac{\Delta S_H}{R}; R \text{ is the ideal gas constant, } \Delta H_H = 42 \pm 22 \text{ kJ/mol, } \Delta S_H = 0.11 \pm 0.08 \text{ kJ/mol-K} \]

—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.48, 5.66, 5.98, 5.71</td>
<td>(RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
</tr>
<tr>
<td>5.872</td>
<td>(slow stirring-GC, De Bruijn et al. 1989; De Bruijn &amp; Hermens 1990)</td>
</tr>
<tr>
<td>5.71</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>5.87</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.52, 8.52</td>
<td>(0, 20°C, multi-column GC-k’ correlation; Zhang et al. 1999)</td>
</tr>
<tr>
<td>8.03</td>
<td>(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log \( BCF \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.79</td>
<td>(oyster, Vreeland 1974; quoted, Hawker &amp; Connell 1986)</td>
</tr>
<tr>
<td>3.79, 6.04</td>
<td>(oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
</tr>
<tr>
<td>4.57, 5.87</td>
<td>(fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
</tr>
</tbody>
</table>

Partition Coefficient between particulate and dissolved contaminant concentrations, log \( K_p \) or log \( K_d \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.80</td>
<td>(Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log \( K_{OC} \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.26</td>
<td>(suspended particulate matter, Burkhard 1984)</td>
</tr>
<tr>
<td>4.64</td>
<td>(soil, calculated-S, Chou &amp; Griffin 1986)</td>
</tr>
<tr>
<td>5.80</td>
<td>(average, colloids and micro-particulates in precipitation events, GC/ECD, Murray &amp; Andren 1992)</td>
</tr>
<tr>
<td>5.20</td>
<td>(soil, calculated-( K_{ow} ), Girvin &amp; Scott 1997)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) as or indicated: *data at other temperatures see reference: \( k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^-1 \text{ s}^-1 \) for trichlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 14–30 \text{ d}, due to gas-phase loss process at room temp. (Atkinson 1987) \( k_{OH}(\text{aq.}) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^-1 \text{ s}^-1 \), PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from \( t_{1/2} \approx 4–11 \text{ d} \) in freshwater systems, \( t_{1/2} = 0.1–10 \text{ d} \) in cloud water, \( t_{1/2} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991) \( k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^-1 \text{ s}^-1 \) for trichlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 6.9–15 \text{ d} \) at room temp. (Kwok et al. 1995)
Biodegradation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4–11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1–10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants $k_d$ for labile PCBs sorbed to utility substation soils are: $k = 1.90 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.88 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.37 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants $k_d$ for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00413 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00099 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00052 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 88 \text{ d}$ for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.34 2,3',5'-Trichlorobiphenyl (PCB-34)

![Chemical Structure](image)

Common Name: 2,3',5'-Trichlorobiphenyl  
Synonym: PCB-34, 2,3',5'-trichlorobiphenyl, 2,3',5'-trichloro-1,1'-biphenyl  
Chemical Name: 2,3',5'-trichlorobiphenyl  
CAS Registry No: 37680-68-5  
Molecular Formula: C_{12}H_{3}Cl_{7}  
Molecular Weight: 257.543

Melting Point (°C):  
58.0  
(Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
247.3  
(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}}$ = 56 J/mol K), F: 0.474 (mp at 58°C)

Water Solubility (g/m³ or mg/L at 25°C):  
0.319  
(S'L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.129  
(RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
0.162  
(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.205  
(calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
0.036  
(P'L supercooled liquid, Burkhard et al. 1985a)
0.0177  
(GC-RI correlation, Burkhard et al. 1985b)
0.0447  
(supercooled liquid P'L, GC-RI correlation, Fischer et al. 1992)
log (P'L/Pa) = –4075/(T/K) + 12.37 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
29.08  
(calculated-P/C, Burkhard 1984)
51.17  
(calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
42.73  
(calculated-QSPR, Dunnivant et al. 1992)
29.0  
(predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{\text{AW}} = -\Delta H_{R}/RT + \Delta S_{R}/R$; R is the ideal gas constant, $\Delta H_{R} = 41 \pm 4$ kJ/mol, $\Delta S_{R} = 0.10 \pm 0.01$ kJ/mol·K  
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:  
5.51  
(calculated-TSA, Burkhard 1984)
5.66  
(calculated-TSA, Hawker & Connell 1988a; quoted, Hanch et al. 1995)
5.71  
(RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988; recommended, Sangster 1993)
5.6522  
(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{\text{oa}}$:  
7.72  
(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $\text{BCF or log } K_{b}$:
Sorption Partition Coefficient, log $K_{OC}$:
5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volutilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9-15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.35 3,3',4-Trichlorobiphenyl (PCB-35)

Common Name: 3,3',4-Trichlorobiphenyl
Synonym: PCB-35
Chemical Name: 3,3',4-trichlorobiphenyl
CAS Registry No: 37680-69-6
Molecular Formula: C_{12}H_{7}Cl_{3}
Molecular Weight: 257.543
Melting Point (°C):
87.0 (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm³):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.301 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0152 (quoted-3,4,4'-trichlorobiphenyl from Weil et al. 1974; Opperhuizen et al. 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00246 (GC-RI correlation, Burkhard et al. 1985a)
0.00949 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.014, 0.0105 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0129 (supercooled liquid P_L; GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4242/(T/K) + 12.37 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
8.13 (calculated-P/C, Burkhard et al. 1985b)
22.49 (calculated-MCI χ, Sabljeic & Güsten 1989)
18.23 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
In K_{AW} = –ΔH_{f}RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 54 ± 3 kJ/mol, ΔS_{f} = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
5.53 (calculated-TSA, Burkhard 1984)
5.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7151 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{oa}:
8.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{oc}$:
5.33 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO3}}$ with NO$_3$ radical and $k_{\text{O3}}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{\text{OH}}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14–30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{\text{OH}}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9–15 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:
### 7.1.1.36 3,3′,5-Trichlorobiphenyl (PCB-36)

![Chemical Structure](image)

**Common Name:** 3,3′,5-Trichlorobiphenyl  
**Synonym:** PCB-36, 3,3′,5-trichloro-1,1′-biphenyl  
**Chemical Name:** 3,3′,5-trichlorobiphenyl

**CAS Registry No:** 38444-87-0  
**Molecular Formula:** C₁₂H₃Cl₇  
**Molecular Weight:** 257.543

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>46 (estimated, Abramowitz &amp; Yalkowsky)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>247.3 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ( \Delta H_{\text{ fus}} ) (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ( \Delta S_{\text{ fus}} ) (J/mol K)</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ( \Delta S_{\text{ fus}} = 56 ) J/mol K), F:</td>
<td></td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C):</td>
<td>0.260 (supercooled liquid Sₘ, calculated-TSA, Burkhard et al. 1985a)</td>
</tr>
<tr>
<td></td>
<td>0.00469, 0.0155, 0.010 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
</tr>
<tr>
<td></td>
<td>0.0814 (calculated-TSA and mp, Abramowitz &amp; Yalkowsky 1990)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C and reported temperature dependence equations):</td>
<td>0.0141 (P_l supercooled liquid, Burkhard et al. 1985a)</td>
</tr>
<tr>
<td></td>
<td>0.0149 (GC-RI correlation, Burkhard et al. 1985b)</td>
</tr>
<tr>
<td></td>
<td>0.0191 (supercooled liquid P_l, GC-RI correlation, different stationary phases, Fischer et al. 1992)</td>
</tr>
<tr>
<td></td>
<td>( \log (P_l/P_a) = -4242/(T/K) + 2.48 ) (GC-RT correlation, supercooled liquid, Falconer &amp; Bidleman 1994)</td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa-m³/mol at 25°C or as indicated):</td>
<td>13.98 (calculated-P/C, Burkhard et al. 1985a)</td>
</tr>
<tr>
<td></td>
<td>51.47 (calculated-molecular connectivity indices, Sabljic &amp; Güsten 1989)</td>
</tr>
<tr>
<td></td>
<td>17.40 (wetted-wall column-GC/ECD, Brunner et al. 1990)</td>
</tr>
<tr>
<td></td>
<td>34.10 (calculated-QSPR, Dunnivant et al. 1992)</td>
</tr>
<tr>
<td></td>
<td>20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)</td>
</tr>
<tr>
<td>( \ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R ); ( \Delta H_{\text{fus}} = 54 \pm 3 ) kJ/mol, ( \Delta S_{\text{fus}} = 0.14 \pm 0.01 ) kJ/mol·K</td>
<td></td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, ( \log K_{\text{OW}} ):</td>
<td>5.57 (calculated-TSA, Burkhard 1984)</td>
</tr>
<tr>
<td></td>
<td>4.15 (RP-HPLC-k′ correlation, Rapaport &amp; Eisenreich 1984)</td>
</tr>
<tr>
<td></td>
<td>5.70 (selected, Shiu &amp; Mackay 1986)</td>
</tr>
<tr>
<td></td>
<td>5.88 (calculated-TSA, Hawker &amp; Connell 1988a; quoted, Hansch et al. 1995)</td>
</tr>
<tr>
<td></td>
<td>5.76, 5.86, 5.80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
</tr>
<tr>
<td></td>
<td>5.81 (recommended, Sangster 1993)</td>
</tr>
<tr>
<td></td>
<td>5.8293 (calculated-molecular properties MNDO-AM1 method, Makino 1998)</td>
</tr>
<tr>
<td>Octanol/Air Partition Coefficient, ( \log K_{\text{OA}} ):</td>
<td>8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)</td>
</tr>
</tbody>
</table>
Bioconcentration Factor, log BCF or log K_d:

Sorption Partition Coefficient, log K_OC:

5.37 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

Volatileization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime}\n\tau(calc) = 14–30 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)} \n\kappa_{OH}(calc) = (1.0 – 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime}
\tau(calc) = 6.9–17 \text{ d at room temp. (Kwok et al. 1995)}

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.37 3,4,4’-Trichlorobiphenyl (PCB-37)

![Chemical Structure of 3,4,4'-Trichlorobiphenyl]

Common Name: 3,4,4’-Trichlorobiphenyl
Synonym: PCB-37
Chemical Name: 3,4,4’-trichlorobiphenyl
CAS Registry No: 38444-90-5
Molecular Formula: C_{12}H_{7}Cl_{3}
Molecular Weight: 257.543
Melting Point (°C): 86.8–87.8 (Weingarten 1961)
Boiling Point (°C): 198.7 (Ruelle & Kesselring 1997)
Density (g/cm³ at 20°C): 1.2024
Molar Volume (cm³/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.244 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0152 (generator column-GC/ECD, Weil et al. 1974)
0.135 (calculated-TSA, Mackay et al. 1980)
0.296 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
0.0853 (calculated-fragment solubility constants, Wakita et al. 1986)
0.072 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0110, 0.0142, 0.00853, 0.853 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0408 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0287 (calculated-QSAR, Dunnivant et al. 1992)
0.0437, 0.115 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.170 (calculated-mp and K_{ow}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0566, 0.00897, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0084 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0127, 0.0094 (supercooled P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00454 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00912, 0.0115 (supercooled liquid P_{L}: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = -4242/(T/K) + 12.33 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0612 (P_{L}, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
84.21 (batch stripping, Atlas et al. 1982)
7.34 (calculated-P/C, Burkhard et al. 1985b)
15.40 (20°C, calculated-P/C, Murphy et al. 1987)
14.59 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
15.41 (calculated-QSAR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H/RT + \Delta S/R; \text{ R is the ideal gas constant, } \Delta H = 54 \pm 3 \text{ kJ/mol, } \Delta S = 0.14 \pm 0.01 \text{ kJ/mol-K} \]

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 5.90 (RP-TLC-\( k' \) correlation, Bruggeman et al. 1982)
- 6.00 (calculated-fragment const., Yalkowsky et al. 1983)
- 5.53 (calculated-TSA, Burkhard 1984)
- 4.94 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.58, 5.86, 5.84, 5.85 (RP-HPLC-\( k' \) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.83 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 5.78 (recommended, Sangster 1993)
- 5.7373 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log \( K_{oa} \):

- 8.97 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 4.58, 5.90 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log \( K_p \) or log \( K_d \):

- 5.70, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log \( K_{oc} \):

- 5.33 (suspended particulate matter, Burkhard 1984)
- 4.81 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 4.81 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 4.46 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with \( NO_3 \) radical and \( k_{O_3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference:

\[ k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 14–30 \text{ d, due to gas-phase loss process at room temp.} \]

(Atkinson 1987)

\[ k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 6.9–15 \text{ d at room temp.} \]

(Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:
7.1.1.38 3,4,5-Trichlorobiphenyl (PCB-38)

Common Name: 3,4,5-Trichlorobiphenyl
Synonym: PCB-38, 3,4,5-trichloro-1,1′-biphenyl
Chemical Name: 3,4,5-trichlorobiphenyl
CAS Registry No: 53555-66-1
Molecular Formula: C₁₂H₃Cl₇
Molecular Weight: 257.543
Melting Point (°C): 114 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$:

Water Solubility (g/m³ or mg/L at 25°C):
0.353 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0104 (Pₗ supercooled liquid, Burkhard et al. 1985a)
0.0566, 0.0111, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
7.62 (calculated-P/C, Burkhard 1984)
20.97 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
2.027 (wetted-wall column-GC/ECD, Brunner et al. 1990)
23.54 (calculated-QSPR, Dunnivant et al. 1992)
19.30 (calculated-QSPR, Achman et al. 1993)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{fus}} = 54 \pm 3$ kJ/mol, $\Delta S_{\text{fus}} = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
5.48 (calculated-TSA, Burkhard 1984)
5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7298 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:
8.92 (calculated-QSAR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{\text{B}}$:

Sorption Partition Coefficient, log $K_{\text{OC}}$:
5.28 (suspended particulate matter, cal-$K_{\text{OW}}$, Burkhard 1984)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Volatileization:**

**Photolysis:**

**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.7–1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14–30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (1.0–2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9–15$ d at room temp. (Kwok et al. 1995)

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

**Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

Half-Lives in the Environment:

**Air:** calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

**Surface water:**

**Ground water:**

**Sediment:**

**Soil:**

**Biota:**
7.1.1.39 3,4',5-Trichlorobiphenyl (PCB-39)

Common Name: 3,4',5-Trichlorobiphenyl
Synonym: PCB-39, 3,4',5-trichloro-1,1'-biphenyl
Chemical Name: 3,4',5-trichlorobiphenyl
CAS Registry No: 38444-88-1
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 257.543
Melting Point (°C):
  88  (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  247.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m³ or mg/L at 25°C):
  0.353  (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
  0.0258  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
  0.0310  (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.0125  (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.0135, 0.00314, 0.00419  (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.0203, 0.0174  (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = –4242/(T/K) + 12.53 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
  12.56  (calculated-P/C, Burkhard et al. 1985a)
  43.57  (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
  30.32  (calculated-QSPR, Dunnivant et al. 1992)
  20.3  (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fR}/RT + ΔS_{fR}/R; R is the ideal gas constant, ΔH_{fR} = 54 ± 3 kJ/mol, ΔS_{fR} = 0.14 ± 0.01 kJ/mol·K
  (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
  5.58  (calculated-TSA, Burkhard 1984)
  5.89  (calculated-TSA, Hawker & Connell 1988a quoted, Hansch et al. 1995)
  5.8173  (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
  8.79  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{BF}:

Sorption Partition Coefficient, log K_{OC}:
  5.38  (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

**Volatileization:**

**Photolysis:**

**Oxidation:** rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO\(_3\) radical and \( k_{O_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:

\[
k_{OH}(\text{calc}) = (0.7–1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 14–30 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}
\]

\[
k_{OH}(\text{calc}) = (1.0–2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for trichlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 6.9–15 \text{ d at room temp. (Kwok et al. 1995)}
\]

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

**Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):**

**Half-Lives in the Environment:**

**Air:** calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

**Surface water:**

**Ground water:**

**Sediment:**

**Soil:**

**Biota:**
7.1.1.40  2,2′,3,3′-Tetrachlorobiphenyl (PCB-40)

![Chemical structure of 2,2′,3,3′-Tetrachlorobiphenyl](image)

**Common Name:** 2,2′,3,3′-Tetrachlorobiphenyl  
**Synonym:** PCB-40  
**Chemical Name:** 2,2′,3,3′-tetrachlorobiphenyl  
**CAS Registry No:** 38444-93-8  
**Molecular Formula:** C₁₂H₆Cl₄  
**Molecular Weight:** 291.988  
**Melting Point (°C):** 119.5–121.5 (Wallnöfer et al. 1973; Hutzinger et al. 1974; Erickson 1986)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):** 1.2024  
**Molar Volume (cm³/mol):**  
- 268.2 (calculated-Le Bas method at normal boiling point)  
- 211.6 (Ruelle & Kesselring 1997)  
**Enthalpy of Fusion, ΔH_fus (kJ/mol):**  
**Entropy of Fusion, ΔS_fus (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:** 0.113 (Shiu & Mackay 1986)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
- 0.034 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)  
- 0.070, 0.0583, 0.0232, 0.0385 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
- 0.0156 (generator column-GC/ECD; Dunnivant & Elzerman 1988)  
**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
- 0.0098 (supercooled liquid Pₜ, GC-RT correlation, Bidleman 1984)  
- 0.00134 (GC-RI correlation, Burkhard et al. 1985a)  
- 0.0112 (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al.)  
- 0.00887, 0.00861 (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
- 0.00255; 0.0020 (selected solid Pₛ; supercooled liquid Pₜ, Shiu & Mackay 1986)  
- 0.00452 (20°C, supercooled liquid Pₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)  
- log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)  
- 0.00676, 0.012 (supercooled liquid Pₜ; GC-RI correlation, different stationary phases, Fischer et al. 1992)  
- log (Pₜ/Pa) = –4271/(T/K) + 12.32 (supercooled liquid Pₜ, GC-RT correlation, Falconer & Bidleman 1994)  
- 0.000473–0.00957; 0.00450–0.0120 (literature Pₛ range; literature Pₜ range, Delle Site 1997)  
**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):**  
- 20.27 (calculated-P/C, Burkhard et al. 1985b)  
- 12.16 (20°C, batch stripping-GC, Oliver 1985)  
- 21.94 (calculated-P/C, Shiu & Mackay 1986)  
- 16.31 (20°C, calculated-P/C, Murphy et al. 1987)  
- 20.47 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)  
- 10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)  
- 18.52 (calculated-QSAR, Dunnivant et al. 1992)  
29.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\[ \ln K_{\text{AW}} = -\Delta H_{\text{f}}/R + \Delta S_{\text{f}}/R \]; R is the ideal gas constant, \( \Delta H_{\text{f}} = 30 \pm 3 \text{ kJ/mol} \), \( \Delta S_{\text{f}} = 0.06 \pm 0.01 \text{ kJ/mol-K} \)

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
- 4.63 (HPLC-RT correlation, Sugiura et al. 1978)
- 5.56 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.80 (shake flask-GC, Chiou 1985)
- 5.48, 5.66, 5.84, 5.85 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.55 (generator column-GC/ECD, Hawker & Connell 1988a)
- 6.178 (slow stirring-GC; De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 5.67 (recommended, Sangster 1993)
- 6.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
- 8.05 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- 3.08 (killifish, Goto et al. 1978)
- 3.36–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
- 4.69, 4.23; 5.38 (rainbow trout: laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
- 4.38, 4.23 (worms, fish, Oliver 1987c)
- 4.23 (fish, quoted, Isnard & Lambert 1988, 1989)

Bioaccumulation Factor, log BAF:
- 6.48 (rainbow trout, L/kg(Ip), quoted, Thomann 1989)

Biota Sediment Accumulation Factor, BSAF:
- 10 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log \( K_{OC} \):
- 5.57 (suspended particulate matter, Burkhard 1984)
- 5.50; 5.50 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
- 5.00 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
- 5.00 (soil, calculated-\( K_{OW} \), Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, \( t_1/2 \):
- Volatilization:
  - Photolysis:
  - Hydrolysis:
  - Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3 or as indicated, *data at other temperatures see reference:
    - \( k_{OH}(\text{calc}) = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 25–60 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
    - \( k_{OH}(\text{aq.}) = 6.1 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \), PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
    - \( k_{OH}(\text{calc}) = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 8.5–40 \text{ d} \) at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_2 = 0.0065$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
- $k_1 = 320$ d$^{-1}$; $k_2 = 0.0065$ d$^{-1}$ (rainbow trout, Oliver & Niimi 1985)
- $\log 1/k_2 = 2.2, 2.9$ h (fish, quoted, calculated-$K_{OW}$, Hawker & Connell 1988b)
- $k_2 = 0.006$ d$^{-1}$ with $t_{1/2} = 107$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.006$ d$^{-1}$ with $t_{1/2} = 112$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:
Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants $k_d$ for labile PCBs sorbed to utility substation soils are: $k = 0.20$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.95$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.36$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants $k_d$ for nonlabile PCBs sorbed to utility substation soils are; $k = 0.00155$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00285$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00258$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00119$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: half-life in rainbow trout, $t_{1/2} = 107$ d and $t_{1/2} = 61$ d its muscle (Niimi & Oliver 1983); $t_{1/2} = 107$d in rainbow trout (Oliver & Niimi 1985); $t_{1/2} = 29$ d in worms at 8°C (Oliver 1987c).

depuration $t_{1/2} = 107$ d for high-dose treatment, $t_{1/2} = 112$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.41 2,2′,3,4-Tetrachlorobiphenyl (PCB-41)

Common Name: 2,2′,3,4-Tetrachlorobiphenyl
Synonym: PCB-41, 2,2′,3,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4-tetrachlorobiphenyl
CAS Registry No: 52663-59-9
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988
Melting Point (°C):
63 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.150 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0648 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.0306, 0.0328, 0.0197, 0.0351 (RP-HPLC-k'' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0124 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0131 (GC-RI correlation, Burkhard et al. 1985b)
0.0110, 0.0098 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.59 × 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0776, 0.0120 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/P_a) = −4229/(T/K) + 12.22 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
23.91 (calculated-P/C, Burkhard et al. 1984)
20.37 (calculated-P/C, Murphy et al. 1987)
20.87 (calculated-molecular-connectivity indices, Sabljic & Güsten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)
24.76 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_{f}^{°}/RT + ΔS_{f}^{°}/R; R is the ideal gas constant, ΔH_{f} = 27 ± 2 kJ/mol, ΔS_{f} = 0.05 ± 0.01 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
5.09, 6.11 (RP-HPLC-k’ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.73, 5.83, 5.82, 5.78 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (recommended, Sangster 1993)
6.11 (recommended, Hansch et al. 1995)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 9.79, 8.82 (0, 20°C, RP-HPLC-RT, Zhang et al. 1999)
- 8.46 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:
Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
- 5.80, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log $K_{OC}$:
- 5.59 (suspended particulate matter, Burkhard 1984)
- 5.01 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 5.40 (soil-organic carbon, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Vaporization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{N\text{O}_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}(\text{aq.}) = 6.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.005 \text{ d}^{-1}$ with $t_\frac{1}{2} = 147 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_\frac{1}{2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_\frac{1}{2} \sim 4–11 \text{ d}$ in freshwater systems, $t_\frac{1}{2} = 0.1–10 \text{ d}$ in cloud water, $t_\frac{1}{2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_\frac{1}{2} = 147 \text{ d}$ for high-dose treatment, $t_\frac{1}{2} = 162 \text{ d}$ for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.42 2,2′,3,4′-Tetrachlorobiphenyl (PCB-42)

Common Name: 2,2′,3,4′-Tetrachlorobiphenyl
Synonym: PCB-42, 2,2′,3,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′-tetrachlorobiphenyl
CAS Registry No: 36559-22-5
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C):
69.0 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
Boiling Point (°C):

Density (g/cm³):
268.2 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.370 (mp at 69°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.150 (supercooled liquid S_{L}, calculated-TSA, Burkhard et al. 1985a)
0.0608 (20°C, supercooled liquid S_{L}, Murphy et al. 1987)
0.032 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0334 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0131 (P_{L} supercooled liquid S_{L}, calculated-GC-RT correlation, Burkhard et al. 1985a)
0.00507 (GC-Rl correlation, Burkhard et al. 1985b)
0.0116, 0.0116 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.19 × 10⁻¹ (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00912, 0.0135 (supercooled liquid P_{L}: GC-Rl correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = –4229/(T/K) + 12.25 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
29.49 (calculated-P/C, Burkhard et al. 1985a)
32.02 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990)
25.92 (calculated-QSPR, Dunnivant et al. 1995)
10.13 (calculated-QSPR, Achman et al. 1993)
38.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 26 ± 3 kJ/mol, ΔS_{f} = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hanchs et al. 1995)
5.72 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
5.72 (quoted values; recommended, Sangster 1993)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.19 (10°C, estimated, Thomas et al. 1998)
8.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.64 (suspended particulate matter, Burkhard 1984)
5.30 (soil-organic carbon, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 – 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 0.006$ d$^{-1}$ with $t_\frac{1}{2} = 123$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d$^{-1}$ with $t_\frac{1}{2} = 140$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants $k_d$ for labile PCBs sorbed to utility substation soils are: $k = 0.20$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.89$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.23$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.35$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants $k_d$ for nonlabile PCBs sorbed to utility substation soils are; $k = 0.00066$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00309$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.0016$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00101$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_\frac{1}{2} = 123$ d for high-dose treatment, $t_\frac{1}{2} = 140$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.43 2,2′,3,5-Tetrachlorobiphenyl (PCB-43)

Common Name: 2,2′,3,5-Tetrachlorobiphenyl
Synonym: PCB-43
Chemical Name: 2,2′,3,5-tetrachlorobiphenyl
CAS Registry No: 70362-46-8
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C): 42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘₚ (kJ/mol):
Entropy of Fusion, ∆Sₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₘₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.130 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0183 (P₁ supercooled liquid, Burkhard et al. 1985a)
0.0194 (GC-RI correlation, Burkhard et al. 1985b)
0.0166, 0.0191 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0123, 0.0191 (supercooled liquid P₁; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P₁/Pa) = –4229/(T/K) + 12.40 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
41.14 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.94 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K₃ₙₐ = –∆Hᵢ/RT + ∆Sᵢ/R; R is the ideal gas constant, ∆Hᵢ = 27 ± 2 kJ/mol, ∆Sᵢ = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₐₒₜₜ:
5.84 (calculated-TSA, Burkhard 1984)
5.75 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8627 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₒₐ:
8.11 (calculated-QSAR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log Kₙᵢ:
Sorption Partition Coefficient, log Kₒₑ:
5.64 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4-0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36-1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 155$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 188$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 155$ d for high-dose treatment, $t_{1/2} = 188$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.44 2,2',3,5'-Tetrachlorobiphenyl (PCB-44)

Common Name: 2,2',3,5'-Tetrachlorobiphenyl
Synonym: PCB-44
Chemical Name: 2,2',3,5'-tetrachlorobiphenyl
CAS Registry No: 41464-39-5
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988

Melting Point (°C):
46.5–47 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2024
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
0.608 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.170 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.080 (generator column-HPLC/UV, Billington 1982)
0.10 (20°C, supercooled liquid Sₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.08 (generator column-HPLC/UV, Billington et al. 1988)
0.0463, 0.0394, 0.0254, 0.0343 (RP-HPLC-k correlation correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00943 (GC-RI correlation, Burkhard et al. 1985a)
0.0147 (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al. 1985b)
0.0128, 0.013 (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0152 (quoted, Eisenreich 1987)
0.0064 (20°C, supercooled liquid Pₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00955, 0.0151 (supercooled liquid Pₜ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₜ/Pa) = – 4229/(T/K) + 12.29 (supercooled liquid Pₜ, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
79.28 (batch stripping, Atlas et al. 1982)
24.32 (calculated, Murphy et al. 1983)
32.83 (calculated-P/C, Burkhard et al. 1985b)
19.15 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (calculated-QSPR-MCI χ, Sabljic & Gusten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990)
23.32 (calculated-QSPR, Dunnivant et al. 1992)
11.86, 16.02, 21.33, 28.05* ± 0.27, 35.13 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 5.8937 – 3103.2/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
Polychlorinated Biphenyls (PCBs)

\[ K_{AW} = \exp \left[ -\frac{(25.8 \text{kJ mol}^{-1})}{RT} + \frac{(0.049 \text{kJ mol}^{-1} \cdot \text{K}^{-1})}{R} \right] \]
where \( R = 8.314 \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \) and temp range: 4–31°C,
(gas stripping-GC, Bamford et al. 2000)—see Comment by Goss et al. 2004

27.0 (exptl. data, Bamford et al. 2002)

\[ \ln K_{AW} = -\frac{\Delta H_f}{RT} + \frac{\Delta S_f}{R} \]
R is the ideal gas constant, \( \Delta H_f = 26 \pm 2 \text{kJ/mol} \), \( \Delta S_f = 0.05 \pm 0.01 \text{kJ/mol-K} \)
(Bamford et al. 2002)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.67</td>
<td>(calculated-fragment const., Yalkowsky et al. 1983)</td>
</tr>
<tr>
<td>5.84</td>
<td>(calculated-TSA, Burkhard 1984)</td>
</tr>
<tr>
<td>5.81</td>
<td>(RP-HPLC-RT correlation, Rapaport &amp; Eisenreich 1984)</td>
</tr>
<tr>
<td>5.29</td>
<td>(calculated-S, Chou &amp; Griffin 1986)</td>
</tr>
<tr>
<td>5.61, 5.74, 5.79</td>
<td>(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
</tr>
<tr>
<td>5.75</td>
<td>(calculated-TSA, Hawker &amp; Connell 1988b)</td>
</tr>
<tr>
<td>5.88</td>
<td>(calculated-MCI χ, Patil 1991)</td>
</tr>
<tr>
<td>5.73</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>5.81</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>6.20, 6.79–6.67</td>
<td>(calculated-Characteristic Root Index [CRI]; minimum-maximum range, Saçan &amp; Inel 1995)</td>
</tr>
<tr>
<td>5.6625</td>
<td>(calculated-molecular properties MNDO-AM1 method, Makino 1998)</td>
</tr>
<tr>
<td>6.26</td>
<td>(calculated-CLOGP ver. 4, Ran et al. 2002)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, \( \log K_{OA} \) or as indicated and reported temperature dependence equations:

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.36</td>
<td>(fugacity meter/generator column-GC; Kömp &amp; McLachlan 1997a)</td>
</tr>
<tr>
<td>( \log K_{OA} = -6.20 + 4340/(T/K) ); (fugacity meter, temp range 10–43°C, Kömp &amp; McLachlan 1997a)</td>
<td></td>
</tr>
<tr>
<td>9.19</td>
<td>(10°C, estimated, Thomas et al. 1998)</td>
</tr>
<tr>
<td>9.67, 8.71; 8.41</td>
<td>(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)</td>
</tr>
<tr>
<td>8.58</td>
<td>(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, \( \log BCF \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.04</td>
<td>(oyster, Vreeland 1974)</td>
</tr>
<tr>
<td>4.84; 6.37</td>
<td>(zebrafish: log BCFw, wet wt basis; log BCFl, lipid wt basis, Fox et al. 1994)</td>
</tr>
<tr>
<td>4.04, 6.29</td>
<td>(oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
</tr>
<tr>
<td>4.84, 5.37</td>
<td>(zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
</tr>
</tbody>
</table>

Partition Coefficient between particulate and dissolved contaminant concentrations, \( \log K_p \) or \( \log K_d \)

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.60, 4.70</td>
<td>(Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, \( \log K_{OC} \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.64</td>
<td>(suspended particulate matter, Burkhard 1984)</td>
</tr>
<tr>
<td>4.43</td>
<td>(soil, calculated-S, Chou &amp; Griffin 1986)</td>
</tr>
<tr>
<td>5.60</td>
<td>(calculated after Karickhoff et al. 1979, Capel &amp; Eisenreich 1990)</td>
</tr>
<tr>
<td>4.67</td>
<td>(calculated after Schwarzenbach &amp; Westall 1981, Capel &amp; Eisenreich 1990)</td>
</tr>
<tr>
<td>5.05</td>
<td>(soil, calculated-QSPR Characteristic Root Index [CRI], Saçan &amp; Balcióğlu 1996)</td>
</tr>
<tr>
<td>5.40</td>
<td>(soil, calculated-K_{OW}, Girvin &amp; Scott 1997)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with \( \text{OH} \) radical, \( k_{NO_3} \) with \( \text{NO}_3 \) radical and \( k_{O_3} \) with \( \text{O}_3 \) or as indicated, *data at other temperatures see reference:

\[ k_{OH}^{(\text{calc})} = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]
for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau^{(\text{calc})} = 25–60 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH(aq.)} = 5.5 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \text{ PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, } t_{1/2} = 0.1–10 d \text{ in cloud water, } t_{1/2} > 1000 d \text{ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)}

k_{OH(calc)} = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 8.5–40 d \text{ at room temp. (Kwok et al. 1995)}

Biodegradation: 99% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- k_1 = 200 d^{-1}; k_2 = .0461 d^{-1} (Zebrafish, 30-d exposure, Fox et al. 1994)
- k_2 = 0.014 d^{-1} \text{ with } t_{1/2} = 49 d \text{ and } k_2 = 0.018 d^{-1} \text{ with } t_{1/2} = 38 d \text{ for food concn of 18 ng/g and 129 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)}
- k_2 = 0.005 d^{-1} \text{ with } t_{1/2} = 146 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- k_2 = 0.004 d^{-1} \text{ with } t_{1/2} = 175 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from t_{1/2} ~ 4–11 d in freshwater systems, t_{1/2} = 0.1–10 d in cloud water, t_{1/2} > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soilds are: k = 0.23 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.98 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.32 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.38 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00090 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00253 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00161 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00122 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration t_{1/2} = 38–49 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration t_{1/2} = 146 d for high-dose treatment, t_{1/2} = 175 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.45 2,2',3,6-Tetrachlorobiphenyl (PCB-45)

Common Name: 2,2',3,6-Tetrachlorobiphenyl
Synonym: PCB-45, 2,2',3,6-tetrachloro-1,1'-biphenyl
Chemical Name: 2,2',3,6-tetrachlorobiphenyl
CAS Registry No: 70362-45-7
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C): 42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.115 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (RP-HPLC-k' correlation, Brodsky & Ballischmier 1988)
0.292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0398 (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0416 (GC-RI correlation, Burkhard et al. 1985b)
0.0226, 0.0268 (supercooled P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0295 (supercooled liquid P_{L}: GC-RI correlation, Fischer et al. 1992)
log (P_{L}/Pa) = –4117/(T/K) + 12.16 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
101.1 (calculated-P/C, Burkhard 1984)
31.92 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
35.95 (calculated-QSPR, Dunnivant et al. 1992)
12.47 (calculated-QSPR, Achman et al. 1993)
25.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
43.0 (from 11°C expctl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{g}/RT + ΔS_{g}/R; R is the ideal gas constant, ΔH_{g} = 26 ± 2 kJ/mol, ΔS_{g} = 0.05 ± 0.01 kJ/mol·K
(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k’ correlation, Brodsky & Ballischmier 1988)
4.84 (recommended, Sangster 1993)
5.4616 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
8.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 5.68 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O3$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(aq.) = 6.7 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25$^\circ$C, half-lives range from $t_{1/2}$ ~ 4–11 d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
  - $k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 7$ food lipid (mg)/(g worm lipid-d); $k_2 = 0.12$ d$^{-1}$ (earthworm, Wågman et al. 2001)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 175$ d (8$^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 128$ d (8$^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
- Surface water: half-lives range from $t_{1/2} ~ 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
- Ground water:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 6$ d in earthworm given contaminated food (Wågman et al. 2001)
  - depuration $t_{1/2} = 175$ d for high-dose treatment, $t_{1/2} = 128$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8$^\circ$C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.46 2,2′,3,6′-Tetrachlorobiphenyl (PCB-46)

Common Name: 2,2′,3,6′-Tetrachlorobiphenyl
Synonym: PCB-46, 2,2′,3,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,6′-tetrachlorobiphenyl
CAS Registry No: 41464-47-5
Molecular Formula: C12H4Cl4
Molecular Weight: 291.988
Melting Point (°C): 42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C): 
Density (g/cm³): 
Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHfus (kJ/mol): 
Entropy of Fusion, ΔSfus (J/mol K): 
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.114 (Sᵢ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.106 (20°C, supercooled liquid, Murphy et al. 1987)
0.149 (RP-HPLC-k′ correlation, Brodsky & Ballschmieder 1988)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0280 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0272 (Pᵢ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0285 (GC-RI correlation, Burkhard et al. 1985b)
0.0186, 0.0206 (supercooled liquid Pᵢ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.04 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
0.0155 (supercooled liquid Pᵢ: GC-RI correlation, Fischer et al. 1992)
log (Pᵢ/Pₐ) = −4229/(T/K) + 12.37, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
69.81 (calculated-P/C, Burkhard 1984)
26.04 (20°C, calculated-P/C, Murphy et al. 1987)
36.68 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
34.33 (calculated-QSPR, Dunnivant et al. 1992)
18.87 (calculated-QSAR, Achman et al. 1993)
18.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
34.5 (from 11°C expctl. data and compensation point, Bamford et al. 2002)
ln KₘW = −ΔHᵢ/RT + ΔSᵢ/R; R is the ideal gas constant, ΔHᵢ = 28 ± 3 kJ/mol, ΔSᵢ = 0.06 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log Kᵪₒₙₙ:
5.89 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmieder 1988)
5.86 (calculated, Miertus & Jakus 1990)
Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:
- 9.49, 8.56 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1998)
- 7.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \) or \( \log K_b \):

Sorption Partition Coefficient, \( \log K_{OC} \):
- 5.69 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
- Volatilization:
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO3 radical and \( k_{O_3} \) with O3 or as indicated, *data at other temperatures see reference:
  \( k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 25–60 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
  \( k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 8.5–40 \text{ d} \) at room temp. (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
- \( k_2 = 0.006 \text{ d}^{-1} \) with \( t_{1/2} = 112 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.006 \text{ d}^{-1} \) with \( t_{1/2} = 907 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration \( t_{1/2} = 112 \text{ d} \) for high-dose treatment, \( t_{1/2} = 107 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.47 2,2',4,4'-Tetrachlorobiphenyl (PCB-47)

Common Name: 2,2',4,4'-Tetrachlorobiphenyl  
Synonym: PCB-47  
Chemical Name: 2,2',4,4'-tetrachlorobiphenyl  
CAS Registry No: 2437-79-8  
Molecular Formula: C_{12}H_6Cl_4  
Molecular Weight: 291.988

Melting Point (°C):
- 83 (Fichter & Adler 1926; Kühne et al. 1995; Ruelle & Kesselring 1997)
- 41–42 (Hall & Minhaj 1957; Wallnöfer et al. 1973)

Boiling Point (°C):

Density (g/cm³ at 20°C): 1.2024

Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.268 (Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.068 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.990 (supercooled liquid S_{s}, Johnstone et al. 1974)
- 0.0160, 0.0157, 0.0172, 0.0202 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.0541 (22°C, generator column-GC, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.0115 (Neely 1983)
- 0.0111 (GC-RI correlation, Burkhard et al. 1985a)
- 0.0151 (supercooled liquid P_{l}, GC-RI correlation, Burkhard et al. 1985b)
- 0.0152, 0.0156 (supercooled liquid P_{l}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.0115, 0.0162 (supercooled liquid P_{l}; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{l}/Pa) = -4229/(T/K) + 12.37 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
- 42.86 (calculated-P/C, Burkhard et al. 1985b)
- 17.38 (calculated-P/C, Shiu & Mackay 1986)
- 44.48 (calculated-QSAR-χ, Sabljic & Güsten 1989)
- 19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
- 37.30 (calculated-QSPR, Dunnivant et al. 1992)
- 3.05, 8.91 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
- 12.67 (estimated-bond method, EPIWIN v3.04, Hardy 2002)
- 35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

ln K_{AW} = -ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 27 ± 2 kJ/mol, ΔS_{f} = 0.05 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
- 5.68 (shake flask, Tulp & Hutzinger 1978)
- 5.20 (HPLC-k’ correlation, McDuffie 1981)
6.29 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.17 (HPLC-\(k'\) correlation, De Kock & Lord 1987)
5.93, 6.04, 5.86, 5.94 (RP-HPLC-\(k'\) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.94 (recommended, Sangster 1993)
6.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{OA}\) at 25°C or as indicated:
9.55, 8.56 (0, 20°C, multi-column GC-\(k'\) correlation; Zhang et al. 1999)
8.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.98 (rainbow trout muscle, steady state, Branson et al. 1975; quoted, Waid 1986)
4.09 (rainbow trout, Neely et al. 1974)
3.95 (rainbow trout, Branson et al. 1975)
4.85; 4.782, 4.717 (quoted-whole fish; calculated-molecular connectivity indices, \(K_{OW}\) Lu et al. 1999)
2.97, 2.71 (phytoplankton *Nanochloropsis oculata*, PCB concn at 50 ppb, after 4-d culture, Wang et al. 1998)
2.19, 2.11 (phytoplankton *Isochrysis galbana*, PCB concn at 500 ppb, after 4-d culture, Wang et al. 1998)
4.00, 5.52 (rainbow trout 8–10 g, muscle 3% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.46, 5.56 (rainbow trout 10–15 g, whole fish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.76 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log \(K_p\) or log \(K_d\)
5.30, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log \(K_{OC}\):
4.61 (soil, calculated-solubility, Kenaga 1980)
5.72 (suspended particulate matter, calculated-\(K_{OW}\), Burkhard 1984)
4.68 (soil, calculated-S, Chou & Griffin 1986)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.04 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)
5.70 (soil, calculated-\(K_{OW}\), Girvin & Scott 1997)
4.65 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log \(K_p\):
5.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.18–5.64 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k, or Half-Lives, \(t_{1/2}\):
Volatileization: \(t_{1/2} = 0.2921\) d from river, \(t_{1/2} = 9.256\) d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis: photolysis rate \(k_p = 0.553\) d\(^{-1}\) with \(t_{1/2} = 13\) d in summer sunlight; \(k_p(exptl) = 6 \times 10^{-8}\) d\(^{-1}\) with \(t_{1/2} = 133\) d, and \(k_p(calc) = 2.2 \times 10^{-8}\) d\(^{-1}\) in winter sunlight, at 40°L in surface waters (Dulin et al. 1986)
Oxidation: rate constant k, for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO\(_3\) radical and \(k_O3\) with O\(_3\) or as indicated, *data at other temperatures see reference: \(k_{OH}(calc) = (0.4 - 0.9) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) for tetrachlorobiphenyls, and the tropospheric lifetime \(\tau(calc) = 25–60\) d, due to gas-phase loss process at room temp. (Atkinson 1987)
\(k_{OH}(aq.) = 6.4 \times 10^9\) dm\(^3\) mol\(^{-1}\) s\(^{-1}\), PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from \(t_{1/2} \sim 4–11\) d in freshwater systems, \(t_{1/2} = 0.1–10\) d in cloud water, \(t_{1/2} > 1000\) d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
\(k_{OH}(calc) = (0.36 - 1.7) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) for tetrachlorobiphenyls, and the tropospheric lifetime \(\tau(calc) = 8.5–0\) d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: no degradation observed after 98 d incubation by river dieaway test (Bailey et al. 1983).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 286$ d$^{-1}$; $k_2 = 0.030$ d$^{-1}$ (10–12°C, rainbow trout muscle, Branson et al. 1975; quoted, Waid 1986)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 177$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

- Surface water: $t_{1/2} = 49.2$ d in Lake Michigan (Neely 1983);
- photolysis $t_{1/2} = 13$ d in summer sunlight and $t_{1/2} = 170$ d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);
- half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
- half-life of volatilization: $t_{1/2} = 0.2021$ d from river, and $t_{1/2} = 9.156$ d from lake, (estimated-EPIWIN v3.04, Hardy 2002).

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 28$ d in rainbow trout muscle (Branson et al. 1975; selected, Waid 1986).

- depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 177$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.48 2,2′,4,5-Tetrachlorobiphenyl (PCB-48)

Common Name: 2,2′,4,5-Tetrachlorobiphenyl  
Synonym: PCB-48, 2,2′,4,5-tetrachloro-1,1′-biphenyl  
Chemical Name: 2,2′,4,5-tetrachlorobiphenyl  
CAS Registry No: 70362-47-9  
Molecular Formula: C_{12}H_{6}Cl_{4}  
Molecular Weight: 291.988  
Melting Point (°C): 65.9  
(Miller et al. 1984; Ruelle & Kesselring 1997)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol): 268.2  
(calculated-Le Bas method at normal boiling point)  
211.6  
(Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 23.4  
(Miller et al. 1984; Ruelle & Kesselring 1997)  
Entropy of Fusion, ΔS_{fus} (J/mol K): 69.04  
(Miller et al. 1984)  
Fugacity Ratio at 25°C, F: 0.393  
(calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)  
Water Solubility (g/m³ or mg/L at 25°C):  
0.121  
(supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)  
0.030  
(supercooled liquid S_L, Murphy et al. 1987)  
0.0328, 0.0376, 0.0467, 0.0452  
(RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballaschmier 1988)  
0.0923  
(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
0.0222, 0.0596  
(calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
0.0167  
(supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)  
0.0177  
(ÅG, and GC-k correlation, Burkhard et al. 1985b)  
0.0157, 0.016  
(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
0.0265  
(20°C, supercooled liquid, Murphy et al. 1987)  
0.0115, 0.0170  
(supercooled liquid P_L: GC-R1 correlation, different stationary phases, Fischer et al. 1992)  
log (P_L/Pa) = −4229/(T/K) + 12.37  
(GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
0.010  
(P_L, calculated-MCI χ and Characteristic Root Index CRI; Saçan & Balcioglu 1998)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
42.71  
(calculated-P/C, Burkhard et al. 1985b)  
26.64  
(calculated-molecular connectivity indices, Sabljic & Gunsten 1989)  
30.67  
(calculated-QSPR, Dunnivant et al. 1992)  
19.30  
(calculated-QSPR, Achman et al. 1993)  
3.05, 8.91  
(0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)  
22.8  
(11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
39.8  
(from 11°C exp. data and compensation point, Bamford et al. 2002)  
ln K_{AW} = –ΔH_G/RT + ΔS_G/R; R is the ideal gas constant, ΔH_{liq} = 25 ± 2 kJ/mol, ΔS_{liq} = 0.05 ± 0.01 kJ/mol-K  
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 5.86 (calculated-TSA, Burkhard 1984)
- 5.78 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 5.71, 5.79, 5.56 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.95 (calculated-solvatochromic parameters and intrinsic molar volume $V_I$, Kamlet et al. 1988)
- 5.69 (recommended, Sangster 1993)
- 5.9108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 9.49, 8.50 (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
- 8.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
- 4.41, 5.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
- 5.66 (suspended particulate matter, Burkhard 1984)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:
$$k_{OH}(calc) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(cal)= 25$–$60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$$k_{OH}(aq.) = 6.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \text{ PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from } t_{1/2} \sim 4$–$11 \text{ d in freshwater systems, } t_{1/2} = 0.1$–$10 \text{ d in cloud water, } t_{1/2} > 1000 \text{ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)}$$
$$k_{OH}(calc) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(cal)= 8.5$–$40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 160 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)}$
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 177 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)}$

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4$–$11 \text{ d in freshwater systems, } t_{1/2} = 0.1$–$10 \text{ d in cloud water, } t_{1/2} > 1000 \text{ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)}$

Ground water:

Soil:

Biota: depuration $t_{1/2} = 160 \text{ d for high-dose treatment, } t_{1/2} = 177 \text{ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)}$
7.1.1.49 2,2’,4,5’-Tetrachlorobiphenyl (PCB-49)

Common Name: 2,2’,4,5’-Tetrachlorobiphenyl
Synonym: PCB-49, 2,2’,4,5-tetrachlorobiphenyl, 2,2’,4,5’-tetrachloro-1,1’-biphenyl
Chemical Name: 2,2’,4,5’-tetrachlorobiphenyl
CAS Registry No: 41464-40-8
Molecular Formula: C\textsubscript{12}H\textsubscript{6}Cl\textsubscript{4}
Molecular Weight: 291.988
Melting Point (°C):
66.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
23.4 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
69.04 (Miller et al. 1984)
69.01, 64.3 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.392 (mp at 66.5°C)
0.411 (Shiu & Mackay 1986)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
0.0164 (generator column-GC/ECD, Miller et al. 1984,1985)
0.0202, 0.0193, 0.0232, 0.0266 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00708 (GC-RI correlation, Burkhard et al. 1985a)
0.0170 (supercooled liquid P\textsubscript{T}, GC-RI correlation, Burkhard et al. 1985b)
0.0167, 0.0162 (supercooled liquid P\textsubscript{T}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00742 (20°C, supercooled liquid P\textsubscript{T}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.60 - 4440/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0123, 0.0182 (supercooled liquid P\textsubscript{T}, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P/P_{\text{a}}) = -4229/(T/K) + 12.41$ (supercooled liquid P\textsubscript{T}, GC-RT correlation, Falconer & Bidleman 1994)
0.00955 (20°C, supercooled liquid P\textsubscript{T}, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C as indicated):
20.27 (calculated, Murphy et al. 1983)
47.72 (calculated-P/C, Burkhard et al. 1985b)
27.96 (20°C, calculated-P/C, Murphy et al. 1987)
37.90 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.79 (calculated-QSPR, Dunnivant et al. 1992)
22.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{\text{AW}} = -\Delta H_{\text{j}}/RT + \Delta S_{\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{j}} = 25 \pm 2$ kJ/mol, $\Delta S_{\text{fus}} = 0.05 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- $6.23$ (calculated-$\pi$ constant, Bruggeman et al. 1982)
- $5.73$ (generator column-GC/ECD, Miller et al. 1984, 1985)
- $6.22$ (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- $5.96, 5.98, 5.77, 5.86$ (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- $6.361 \pm 0.046; 6.23$ (slow stirring-GC, calculated-$\pi$ const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- $5.87$ (recommended, Sangster 1993)
- $6.38$ (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated and reported temperature dependence equations.
- $8.57$ (20°C, generator column-GC, measured range –10 to 20°C, Harner & Bidleman 1996)
- $9.64, 9.08, 8.57, 8.21$ (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Bidleman 1996)
- $\log K_{oa} = -4.96 + 3981/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
- $9.08$ (10°C, estimated, Thomas et al. 1998)
- $9.50, 8.63; 8.48$ (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- $8.34$ (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- $4.84; 6.37$ (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
- $4.84, 6.38$ (zebrafish, kinetic approach: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{oc}$:
- $5.71$ (suspended particulate matter, calculated-K_{ow}, Burkhard 1984)
- $5.90$ (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- $5.50$ (soil, calculated-K_{ow}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3, or as indicated, *data at other temperatures see reference:
- $k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $t(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}(aq.) = 6.2 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}(calc) = 0.36 – 1.7$ \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $t(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 3200$ d$^{-1}$; $k_2 = 0.0458$ d$^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants $k_d$ for labile PCBs sorbed to utility substation soils are: $k = 0.25$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.99$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.31$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants $k_d$ for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00094$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00243$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00168$ d$^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00147$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{1/2} = 158$ d for high-dose treatment, $t_{1/2} = 196$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.50 2,2',4,6-Tetrachlorobiphenyl (PCB-50)

Common Name: 2,2',4,6-Tetrachlorobiphenyl
Synonym: PCB-50, 2,2',4,6-tetrachloro-1,1'-biphenyl
Chemical Name: 2,2',4,6-tetrachlorobiphenyl
CAS Registry No: 62796-65-8
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988
Melting Point (°C): 45.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   0.092 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
   0.0320, 0.032, 0.030, 0.0412 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
   0.1842 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
   0.044 (calculated-MCI χ, Patil 1991)
Vapor Pressure (Pa at 25°C):
   0.0451 (GC-RI correlation, Burkhard et al. 1985a)
   0.0433 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
   76.80 (gas stripping-GC, Atlas et al. 1982)
   137.8 (calculated-P/C, Burkhard et al. 1985b)
   58.57 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
   61.76 (calculated-QSPR, Dunnivant et al. 1992)
   28.68, 38.18, 49.84, 64.30 ± 1.4, 70.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 5.8937 – 2862.64/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{AW} = \exp[-(23.8/kJ·mol^{-1})/R] + (0.049/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
60.5 (exptl. data, Bamford et al. 2002)
ln K_{AW} = -\Delta H_g/RT + \Delta S_g/R; R is the ideal gas constant, \Delta H_g = 24 ± 4 kJ/mol, \Delta S_g = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
   5.96 (calculated-TSA, Burkhard 1984)
   5.72, 5.84, 5.70, 5.74 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
   5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
   5.87 (calculated-MCI χ, Patil 1991)
   5.75 (recommended, Sangster 1993)
   5.6545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:
7.89 \hspace{7mm} (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.26, 3.50, 3.81 (algae, fish, activated sludge, Freitag et al. 1984, 1985)

Sorption Partition Coefficient, log $K_{OC}$:
5.76 \hspace{7mm} (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  \[ k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  \[ k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

- Biodegradation:
- Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
7.1.1.51 2,2′,4,6′-Tetrachlorobiphenyl (PCB-51)

Common Name: 2,2′,4,6′-Tetrachlorobiphenyl
Synonym: PCB-51
Chemical Name: 2,2′,4,6′-tetrachlorobiphenyl
CAS Registry No: 68194-04-7
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988

Melting Point (°C): 66 (Brodsky & Ballschmitter 1988)
Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 0.396 (mp at 66°C)

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

Henry’s Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

5.76 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 10 \text{ food lipid (mg)/(g worm lipid-d)}$; $k_2 = 0.11 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 126 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 150 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 6 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 126 \text{ d}$ for high-dose treatment, $t_{1/2} = 150 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.52 2,2′,5,5′-Tetrachlorobiphenyl (PCB-52)

Common Name: 2,2′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-52
Chemical Name: 2,2′,5,5′-tetrachlorobiphenyl
CAS Registry No: 35693-99-3
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C):
87–89 (Webb & McCall 1972; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2024
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point.)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
46.02 (Hinckley et al. 1990)
46.1 (Passivirta et al. 1999)
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

© 2006 by Taylor & Francis Group, LLC
0.0104 (supercooled liquid $P_L$, converted from literature $P_S$ with $\Delta S_{\text{ fus}}$; Bidleman 1984)
0.0159, 0.0229 (supercooled liquid $P_L$, calculated from $P_{GC}$; GC-RT correlation, different stationary phases, Bidleman 1984)
0.00492 (GC-RI correlation, Burkhard et al. 1985a)
0.00497; 0.0193 (selected $P_S$, supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985)
0.0184, 0.0173 (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0049; 0.0020 (selected solid $P_S$, supercooled liquid $P_L$, Shiu & Mackay 1986)
0.00904 (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0127; 0.0546 (calculated-S X HLC; solid $P_S$, supercooled liquid $P_L$, Dunnivant & Elzerman 1988)
log ($P/mmHg) = 10.60 – 4430/(T/K)$ (GC-RT correlation, supercooled liquid, Tateya et al. 1988)
0.0104, 0.008 (supercooled $P_L$, converted from literature $P_S$ with different $\Delta S_{\text{ fus}}$ values, Hinckley et al. 1990)
0.0188, 0.012 (P$_{GC}$ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log ($P_L/Pa) = 11.74 – 4127/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
0.0132, 0.020 (supercooled liquid $P_L$; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log ($P_L/Pa) = – 4220/(T/K) + 12.36$ (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)
0.00690; 0.00218 (solid $P_S$, supercooled liquid $P_L$, Passivirta et al. 1999)
log ($P_L/Pa) = 14.77 – 5087/(T/K)$ (solid, Passivirta et al. 1999)
log ($P_L/Pa) = 12.36 – 4220/(T/K)$ (liquid, Passivirta et al. 1999)
0.0033–0.013; 0.00901–0.0512 (literature $P_S$ range; literature $P_L$ range, Delle Site 1997)
0.00904 (supercooled liquid $P_L$, calculated-MCI $\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0107, 0.0120 (supercooled liquid $P_L$; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log ($P_L/Pa) = –4190/(T/K) + 12.08$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
log ($P_L/Pa) = –4059/(T/K) + 11.69$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry’s Law Constant (Pa m$^3$/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
31.41–53.7 (calculated-P/C, Westcott et al. 1981)
14.1–53.7 (calculated-P/C, Westcott & Bidleman 1981)
94.15 (gas stripping-GC/ECD, Atlas et al. 1982)
22.29 (calculated-P/C, Murphy et al. 1983)
26.34 (calculated-P/C, Murphy 1984)
31.41–53.70 (calculated-P/C, Bidleman 1984)
53.20 (calculated-P/C, Burkhard et al. 1985b)
2.53 (batch stripping-GC, Hassett & Milicic 1985)
12.16 (20°C, gas stripping-GC, Oliver 1985)
47.59 (calculated-P/C, Shiu & Mackay 1986)
24.11 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
34.65 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
44.04 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.34 (calculated-QSPR, Dunnivant et al. 1992)
16.4* (20°C, gas stripping-HPLC/fluorescence, measured range 10–48°C, ten Hulscher et al. 1992)
17.0 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
log [H/(Pa m$^3$/mol)] = 13.15 – 3552/(T/K) (Passivirta et al. 1999)
31.07* ± 0.42 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$K_{\text{AW}} = \exp[-(30.5/(kJ-mol^{-1}•K^{-1})/R)]$; where $R = 8.314$ J K$^{-1}$ mol$^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
28.27 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 2001)
log $K_{\text{AW}} = 6.427 – 2530/(T/K)$ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
31.3 (exptl. data, Bamford et al. 2002)
ln $K_{\text{AW}} = –\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{fus}} = 31 ± 3$ kJ/mol, $\Delta S_{\text{fus}} = 0.07 ± 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
28.18, 25.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
Polychlorinated Biphenyls (PCBs)

log \([H/(\text{Pa m}^3/\text{mol})] = -2189/(T/\text{K}) + 8.79\) (LDV linear regression of literature data, Li et al. 2003)
log \([H/(\text{Pa m}^3/\text{mol})] = -2956/(T/\text{K}) + 11.32\) (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
- 3.91 (shake flask-radiolabeled-\(^{14}\)C-LSC, Metcalf et al. 1975)
- 5.81 (Hansch & Leo 1979)
- 6.26 (RP-TLC-k' correlation, Bruggeman et al. 1982)
- 6.09 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.81, 5.87, 5.43, 5.80 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.02 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
- 5.81 (generator column-GC, Larsen et al. 1992)
- 6.00 (HPLC-k' correlation, Noegrohati & Hammers 1992)
- 5.79 (recommended, Sangster 1993)
- 6.09 (recommended, Hansch et al. 1995)
- 6.10 (calculated, Passivirta et al. 1999)
- 6.00, 5.91 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\) or as indicated and reported temperature dependence equations:
- 7.90 (calculated-\(K_{\text{OW}}/K_{\text{AW}}\), Wania & Mackay 1996)
- 8.22; 7.73 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- log \(K_{\text{OA}} = -6.20 + 4340/(T/\text{K})\); temp range: 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
- 9.10 (10°C, estimated, Thomas et al. 1998)
- 9.46, 8.49; 8.56 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 8.33 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 8.47; 8.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
- 8.22, 8.22 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- log \(K_{\text{OA}} = 4251/(T/\text{K}) – 6.04\) (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log \(B_{\text{CF}}\):
- 3.87 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
- 4.26, 4.60, 4.02, 4.07 (algae, snail, mosquito, fish, Metcalf et al. 1975)
- 2.66 (green sunfish, 15 d in static water, Sanborn et al. 1975)
- 6.21; 6.07 (goldfish, 3% lipid; 10% lipid dry wet in food, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
- 6.38 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984; quoted, Gobas et al. 1987)
- 4.69, 4.98 (goldfish, exptl., correlated, Mackay & Hughes 1984)
- 3.49–4.26 highest value 4.26, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
- 5.30, 4.26; 6.28 (rainbow trout, laboratory data: kinetic BCF (\(k_1/k_2\)), steady state BCF (\(C_F/C_W\)); Lake Ontario field BCF, Oliver & Niimi 1985)
- 4.26, 4.69 (guppy, goldfish, calculated-\(C_{\text{H}}/C_{\text{W}}\) or \(k_1/k_2\), Connell & Hawker 1988; Hawker 1990)
- 6.38; 5.76 (guppy, lipid wt. based, corrected lipid wt. based, Gobas et al. 1989)
- 4.25 (guppy, estimated, Banerjee & Baughman 1991)
- 6.21; 6.32 (lipid basis: goldfish; rainbow trout, Noegrohati & Hammers 1992)
- 4.54, 6.02; 4.782, 4.708 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, \(K_{\text{OW}}\), Lu et al. 1999)
- 3.08–4.58 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.86–6.31 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 5.23 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
- 5.03, 4.67; 3.57, 4.76, 4.17, 5.39 (oligochaetes; chironomid larvae, Bott & Standley 2000)
- 3.36, 5.60 (\textit{Daphnia}, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 3.87, 6.12 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.28, 6.23 (mussel *Mutilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.42, 6.34 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.63, 5.93 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.69, 5.99 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.92, 6.46 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.01; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Bioaccumulation Factor, log BAF at 25°C or as indicated:
- 7.38 (rainbow trout, lipid based-L/kg(Ip), quoted, Thomann 1989)
- 4.92; 6.43 (22°C, zebrafish: log BCFW wet wt basis; log BCFL lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
- 5.60, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.30 (average, colloids and micro-particles in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.73–5.15 (field-generated particulates, New Bedford Harbor; Bergen et al. 1993)

Sorption Partition Coefficient, log $K_{oc}$ at 25°C or as indicated:
- 4.67 (Woodburn soil silt loam, sorption isotherm measurement, Haque & Schmedding 1976)
- 5.91 (suspended particulate matter, calculated-$K_{OM}$, Burkhard 1984)
- 5.60; 5.50; 5.70 (field data of sediment trap material; Niagara River-organic matter; calculated-$K_{OW}$, Oliver & Charlton 1984)
- 4.54, 4.42 (Aldrich humic acid with 9.4 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
- 3.87, 4.36 (Huron River water with 7.8 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
- 4.87 (dissolved humic acid, gas purging-LSC, Hassett & Milicic 1985)
- 5.35 (suspended solids-Lake Superior; field measurement-GC/ECD, Baker et al. 1986)
- 5.70, 4.87 (Lake Superior suspended solids: calculated-KOW, Baker et al. 1986)
- 6.15 (Composite Condine silt soil 0.36% OC, batch sorption equilibrium, Anderson & Pankow 1986)
- 5.0–6.4, 5.9 (suspended sediment, range, average, Oliver 1987a)
- 6.12 (Lake Michigan water column, Swackhader & Armstrong 1987)
- 4.65 (calculated, Bahnick & Doucette 1988)
- 3.48 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
- 4.35 (calculated-polymaleic acid, Chin & Weber 1989)
- 5.88 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 4.88 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.83 (organic carbon from total suspended matter of raw water from Lake Michigan, Eadie et al. 1990)
- 5.00, 3.88 (Aldrich humic acid, natural DOC, reversed-phase separation, Eadie et al. 1990)
- 5.00; 4.38–4.81; 2.89–3.93 (Aldrich humic acid; humic acid from soil & water samples; fulvic acid & dissolved organic matter samples, Jota & Hassett 1991)
- 5.00 (soil, batch sorption equilibrium-GC, Paya-Perez et al. 1991)
- 6.0 (soil, batch sorption equilibrium-GC, Paya-Perez et al. 1991)
- 5.41 (soil, batch sorption equilibrium-GC, Paya-Perez et al. 1991)
- 6.04, 4.80 (Hamlet City lake sediment, WES reference soil, batch sorption equilibrium, Brannon et al. 1995)
- 5.02, 2.64; 4.80 (sediments from Brown’s Lake, Hamlet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
- 5.03, 3.95 (stony, quoted lit.; calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 4.97; 5.09 (soil, quoted lit.; calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 5.30–5.41 (soil-Catlin silt loam, $f_{OC} = 0.0226$, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
- 5.61–5.65 (Cloudland loam, $f_{OC} = 0.0024$, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)
- 5.30–5.31 (Kenoma silt loam, $f_{OC} = 0.0153$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
- 5.38 (Kenoma silt loam, $f_{OC} = 0.0092$, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
- 5.43–5.53 (Kenoma silt loam, $f_{OC} = 0.002$, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
- 5.26–5.44 (Norborne silt loam, $f_{OC} = 0.0137$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
Polychlorinated Biphenyls (PCBs)

5.24–5.36 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.39–5.40 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.50 (soil, calculated-K_{ow}, Girvin & Scott 1997)
5.50; 4.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
4.98 (sediment, Bott & Stanldey 2000)
5.02, 4.55 (soil, calculated-K_{OW}, Girvin & Scott 1997)
5.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
3.79–6.07; 4.40–6.40 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.32; 5.52, 5.38, 5.60 (A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:
4.67 (Haque & Schmedding 1976; Chou & Griffin 1986)
4.67, 4.62 (quoted, calculated-MCI χ, Sabljic 1984)
3.88 (Great Lake DOC, reversed-phase separation, Eadie et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization: t_{1/2}(exptl) = 2.8 h of evaporation from an initial concentration of 0.005 ppm in a glass dish of 4.5 cm depth of water solution at 24°C and t_{1/2} = 0.68 h with stirring of the solution (Chiou et al. 1979); depletion k = 34 d^{-1} from a 26-cm or 67-cm height purge vessels. from aqueous solution (Girvin et al. 1997).

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO3 radical and k_{O3} with O3 as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 25–60 \text{ d}, \text{ due to gas-phase loss process at room temp. (Atkinson 1987)}
k_{OH}(calc) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 8.5–40 \text{ d} \text{ at room temp. (Kwok et al. 1995)}

Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.1 yr^{-1} in the water column and k = 1.0 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:
k_{2} = 0.008 d^{-1} (11°C, rainbow trout, Guiney et al. 1977; quoted, Waid 1986)
k_{2} = 0.003 d^{-1} (10–11°C, rainbow trout eggs and sac fry, Guiney et al. 1980; quoted, Waid 1986)
k_{2} = 740 d^{-1}; k_{2} = 0.015 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
k_{1} = 280 d^{-1}; k_{2} = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_{1} = 1200 d^{-1}; k_{2} = 0.015 d^{-1} (guppy, Bruggeman et al. 1984)
k_{3} = 0.015, 0.0134 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_{1} = 2800 d^{-1}; k_{2} = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_{2} = 30.8 h^{-1}; 1/k_{2} = 0.015 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_{1} = 30.8 h^{-1}; 1/k_{1} = 0.015 d^{-1} (guppy, Bruggeman et al. 1984)
k_{1} = 50.0 h^{-1}; 1/k_{1} = 0.015 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_{1} = 1100 d^{-1} (guppy, Oppenhuizen 1986)

log k_{1} = 2.87 d^{-1}; log 1/k_{2} = 1.2 d (fish, quoted, Connell & Hawker 1988)

log 1/k_{1} = 2.9; 3.0 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)
1/k_{2} = 30.3 d (guppy, quoted, Clark et al. 1990)
1/k_{2} = 61.7; 102 d (guppy, Gobas et al. 1993; quoted, Clark et al. 1990)
k_{1} = 3230 d^{-1}; k_{2} = 0.0387 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_{2} = 0.011 d^{-1} with t_{1/2} = 65 d and k_{1} = 0.018 d^{-1} with t_{1/2} = 39 d for food concn of 22 ng/g and 125 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_{1} = 20 L d^{-1} g^{-1} dry wt.; k_{2} = 0.118 d^{-1} (Baltic Sea blue mussels, flow-through experiment., Gustafsson et al. 1999)
k_1 = 0.00061 h^{-1}; k_2 = 0.0115 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 9 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.09 d^{-1} (earthsworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with t_{1/2} = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with t_{1/2} = 196 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)
k_2 = 0.015 d^{-1} with t_{1/2} = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1996);
t_{1/2} = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: t_{1/2} = 19.7 d in Lake Michigan (Neely 1983);
t_{1/2} = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: t_{1/2} = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.27 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.99 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.30 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.39 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00112 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00251 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00174 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00127 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
t_{1/2} = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: t_{1/2} = 1.76 yr in female rainbow trouts, t_{1/2} = 1.43 yr in males (Guiney et al. 1980);
t_{1/2} = 500 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985); and t_{1/2} = 99 d in its muscle, (Niimi & Oliver 1983);
t_{1/2} = 46 d in guppy (Bruggeman et al. 1984);
t_{1/2} = 43 d in worms at 8°C, 43 d (Oliver 1987c)
depuration t_{1/2} = 39–65 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
theoretical half-life to reach 90% steady-state tissue concn 5.9 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
t_{1/2} = 6.0 h in blood plasma (ring doves, Drouillard & Norstrom 2000)
elimination t_{1/2} = 8 d in earthworm given contaminated food (predicted, Wågman et al. 2001).
depuration t_{1/2} = 158 d for high-dose treatment, t_{1/2} = 196 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration t_{1/2} = 46.2 d for juvenile carp in 100-d experiment (Stapleton et al. 2004)
#### TABLE 7.1.1.52.1
Reported vapor pressures and Henry’s law constants of 2,2′,5,5′-tetrachlorobiphenyl (PCB-52) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas saturation-GC/ECD</td>
<td>gas stripping-GC</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.00253</td>
<td>10.4</td>
<td>8.6</td>
<td>4</td>
<td>11.34</td>
</tr>
<tr>
<td>30</td>
<td>0.0048</td>
<td>20.0</td>
<td>16.4</td>
<td>11</td>
<td>16.13</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30.1</td>
<td>37.4</td>
<td>18</td>
<td>22.56</td>
</tr>
<tr>
<td></td>
<td></td>
<td>34.9</td>
<td>38.8</td>
<td>25</td>
<td>31.07</td>
</tr>
</tbody>
</table>

\[ \log P = A - \frac{B}{T/K} \]

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.8</td>
<td>4920</td>
</tr>
</tbody>
</table>

temp range 30–40°C

log P = A – B/(T/K) m/mHg

A 11.8
B 4920

\[ \ln K_{AW} = -\Delta H/RT + \Delta S/R \]

\[ \Delta H/(kJ\cdot mol^{-1}) = 30.5 \pm 2.8 \]
\[ \Delta S/(J\cdot K^{-1} \cdot mol^{-1}) = 66 \pm 10 \]

\[ T\Delta S_{vol}/(kJ\cdot mol^{-1}) = 57.0 \pm 6 \]
at 20°C

![FIGURE 7.1.1.52.1](image)

Logarithm of vapor pressure and Henry’s law constant versus reciprocal temperature for 2,2′,5,5′-tetrachlorobiphenyl (PCB-52).
### 2,2′,5,6′-Tetrachlorobiphenyl (PCB-53)

[Chemical Structure Image]

**Common Name:** 2,2′,5,6′-Tetrachlorobiphenyl

**Synonym:** PCB-53, 2,2′,5,6′-tetrachloro-1,1′-biphenyl

**Chemical Name:** 2,2′,5,6′-tetrachlorobiphenyl

**CAS Registry No:** 41464-41-9

**Molecular Formula:** C₁₂H₆Cl₄

**Molecular Weight:** 291.988

**Melting Point (°C):**

103–104.5 (Hutzinger et al. 1974)

**Boiling Point (°C):**

**Density (g/cm³):**

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

**Enthalpy of Fusion, ΔH₉₀ (kJ/mol):**

**Entropy of Fusion, ΔS₉₀ (J/mol K):**

**Fugacity Ratio at 25°C (assuming ∆S₉₀ = 56 J/mol K), F:** 0.168 (mp at 104°C)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**

0.0923 (supercooled liquid Sₛ, calculated-TSA, Burkhard et al. 1985b)

0.109 (20°C, supercooled liquid Sₛ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0945, 0.0786, 0.0717, 0.0335 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)

0.0476 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.288 (supercooled liquid Sₛ, calculated-mp, Dunnivant & Elzerman 1988)

0.292 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.044 (calculated-MCI χ, Patil 1991)

0.0520 (calculated-QSPR, Dunnivant et al. 1992)

0.0306 (calculated-group contribution, Kühne et al. 1995)

0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.114 (calculated-mp and K₉₀, Ran et al. 2002)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**

0.00493 (Neely 1983; quoted, Erickson 1986)

0.0273 (supercooled liquid Pₜ, GC-RT correlation, Bidleman 1984)

0.0356 (supercooled liquid Pₜ, GC-RT correlation, Bidleman 1984)

0.0372 (GC-RI correlation, Burkhard et al. 1985a)

0.0356 (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al. 1985b)

0.0268, 0.0331 (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.011 (20°C, supercooled liquid Pₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00671; 0.0405 (calculated-S × HLC, solid Pₛ; supercooled liquid Pₜ, Dunnivant & Elzerman 1988)

log (P/mmHg) = 10.40 – 4310/(T/K) (GC-RT correlation, Tateya et al. 1988)

0.0214, 0.0347 (supercooled liquid Pₜ; GC-RI correlation, different stationary phases, Fischer et al. 1992)


0.0162 (20°C, supercooled liquid Pₜ, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

0.00161–0.0204; 0.0107–0.0385 (literature Pₛ range; literature Pₜ range, Delle Site 1997)

0.00955 (Pₜ, calculated-MCI 3χ and Characteristic Root Index [CRI], reported as 2,2’,5,6- Saçan & Balcioglu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C as indicated):
30.40  (calculated-P/C, Murphy et al. 1983)
112.5  (calculated-P/C, Burkhard et al. 1985b)
28.67  (20°C, calculated-P/C, Murphy et al. 1987)
41.14  (batch stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.26  (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
43.62  (calculated-QSPR, Dunnivant et al. 1992)
17.21  (calculated-QSPR, Achman et al. 1993)
44.8   (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R; \ R \ is \ the \ ideal \ gas \ constant, \ \Delta H_H = 25 \pm 2 \ \text{kJ/mol}, \ \Delta S_H = 0.05 \pm 0.01 \ \text{kJ/mol-K} \]
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):
5.96   (calculated-TSA, Burkhard 1984)
5.90   (calculated-regression analysis with chlorine substituents, Oliver 1987c)
5.39, 5.57, 5.43, 5.80 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballasmiter 1988)
5.46   (generator column-GC, Hawker & Connell 1988a)
5.62   (calculated-TSA, Hawker & Connell 1988a)
5.87   (calculated-MCI \( \chi \), Patil 1991)
5.55   (recommended, Sangster 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
5.98   (quoted, Hansch et al. 1995)
6.12, 5.55–5.90 (calculated-Characteristic Root Index CRI, min.-max. range, Saçan & Inel 1995)
5.4429 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.13   (calculated-CLOGP ver. 4, Ran et al. 2002)
5.67   (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C or as indicated and reported temperature dependence equations.
9.28, 8.70, 8.24, 7.64 (0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
\( \log K_{oa} = -5.26 + 3965/(T/K); \ temp \ range 0–30°C \) (generator column-GC, Harner & Bidleman 1996)
9.18, 8.18; 8.25 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
8.02   (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \):
5.76   (suspended particulate matter, calculated-K\(_{ow}\), Burkhard 1984)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\frac{1}{2} \):
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) as or indicated, *data at other temperatures see reference:
\( k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 25–60 \ \text{d}, \) due to gas-phase loss process at room temp. (Atkinson 1987)
\( k_{OH}(\text{aq.}) = 5.7 \times 10^9 \ \text{dm}^3 \ \text{mol}^{-1} \ \text{s}^{-1}, \) PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from \( t_\frac{1}{2} \approx 4–11 \ \text{d} \) in freshwater systems, \( t_\frac{1}{2} = 0.1–10 \ \text{d} \) in cloud water, \( t_\frac{1}{2} > 1000 \ \text{d} \) in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andre 1991)
\( k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 8.5–40 \ \text{d} \) at room temp. (Kwok et al. 1995)
Biodegradation: 91% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
- \( k₂ = 0.0019 \text{ d}^{-1} \) (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)
- \( k₂ = 0.008 \text{ d}^{-1} \) with \( tₜ₁ = 91 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k₂ = 0.008 \text{ d}^{-1} \) with \( tₜ₁ = 88 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
- Surface water: half-lives range from \( t_{1/2} \approx 4–11 \text{ d} \) in freshwater systems, \( t_{1/2} = 0.1–10 \text{ d} \) in cloud water, \( t_{1/2} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
- Groundwater:
- Sediment:
- Soil:
- Biota: \( t_{1/2} = 365 \text{ d} \) in rainbow trout, \( t_{1/2} = 107 \text{ d} \) in its muscle 107 d (Niimi & Oliver 1983); \( t_{1/2} = 30 \text{ d} \) in worms at 8°C, 30 d (Oliver 1987c).
  - depuration \( t_{1/2} = 91 \text{ d} \) for high-dose treatment, \( t_{1/2} = 88 \text{ d} \) for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.54 2,2′,6,6′-Tetrachlorobiphenyl (PCB-54)

![Chemical structure of 2,2′,6,6′-Tetrachlorobiphenyl](image)

Common Name: 2,2′,6,6′-Tetrachlorobiphenyl  
Synonym: PCB-54, 2,2′,6,6′-tetrachloro-1,1′-biphenyl  
Chemical Name: 2,2′,6,6′-tetrachlorobiphenyl  
CAS Registry No: 15968-05-5  
Molecular Formula: C₁₂H₆Cl₄  
Molecular Weight: 291.988  

Melting Point (°C): 198 (Van Roosmalen 1934; Hutzinger et al. 1974)

Boiling Point (°C):

- Density (g/cm³):
  - 268.2 (calculated-Le Bas method at normal boiling point)
  - 211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \, \text{J/mol K} \)), F: 0.0201 (mp at 198°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

- 0.412, 0.221, 0.143, 0.0882 (RP-HPLC-\( k' \) correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
- 0.0027 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
- 0.0119 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

- 0.0659 (supercooled liquid \( P_L \), Burkhard 1984)
- 0.00132 (GC-RI correlation, Burkhard et al. 1985a)
- 0.0659 (supercooled liquid \( P_L \), GC-RI correlation, Burkhard et al. 1985b)
- 0.0392, 0.0517 (supercooled liquid \( P_L \), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.0566 (supercooled liquid \( P_L \), Dunnivant & Elzerman 1988)
- 0.000227; 0.118 (calculated-\( S \times HLC \), \( P_S \); supercooled liquid \( P_L \), Dunnivant & Elzerman 1988)
- \( \log (P_L/P_a) = -3751/(T/K) + 11.17 \) (supercooled liquid \( P_L \), GC-RT correlation, Falconer & Bidleman 1994)
- 0.000396–0.0219; 0.00388–0.104 (literature \( P_L \) range; literature \( P_S \) range, Delle Site 1997)
- 0.0114 (\( P_L \), calculated-MCI \( \chi \) and Characteristic Root Index [CRI], Saçan & Balcioglu 1998)

Henry’s Law Constant (Pa m³/mol at 25°C):

- 188.5 (calculated-P/C, Burkhard et al. 1985b)
- 15.0 (calculated, Coates & Elzerman 1986)
- 55.73 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
- 50.0 (calculated-QSAR-MCI \( \chi \), Sabljic & Güsten 1989)
- 20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
- 50.04 (calculated-QSPR, Dunnivant et al. 1992)
- 44.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_p/RT + \Delta S_p/R; \text{ R is the ideal gas constant, } \Delta H_p = 25 \pm 2 \, \text{kJ/mol, } \Delta S_p = 0.05 \pm 0.01 \, \text{kJ/mol-K} \] (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 6.63 (calculated after Rekker 1977, Könemann 1981)
- 4.16, 713, 7.01 (HPLC-\( k' \) correlation; calculated-\( \pi \) const.; calculated-fragment const., McDuffie 1981)
5.94 (RP-TLC-retention, Bruggeman et al. 1982)
4.95, 5.27, 5.22, 5.52 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.48 (generator column-GC, Hawker & Connell 1988a)
5.936 ± 0.031 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.24 (recommended, Sangster 1993)
5.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
7.30 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.85; 5.38 (zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.63 (river sediment, Coates & Elzerman 1986)
4.79 (correlated literature values in soils, Sklarew & Girvin 1987)
5.01 (soil, calculated-MCI χ, Sabilje et al. 1995)
5.11; 5.01 (soil, quoted lit.; calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
4.91, 4.84 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4 – 0.9) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau_{(calc)} = 25–60 \text{ d, due to gas-phase loss process at room temp.} \text{ (Atkinson 1987)}
k_{OH}(calc) = (0.36 – 1.7) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau_{(calc)} = 8.5–40 \text{ d at room temp.} \text{ (Kwok et al. 1995)}

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation t_9 = 72.5 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5 kW high pressure Xenon lamp (De Felip et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration t_9 = 190 d for high-dose treatment, t_9 = 100 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.55 2,3,3′,4-Tetrachlorobiphenyl (PCB-55)

Common Name: 2,3,3′,4-Tetrachlorobiphenyl
Synonym: PCB-55, 2,3,3′,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4-tetrachlorobiphenyl
CAS Registry No: 74338-24-2
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988

Melting Point (°C):
89 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
268.2 (calculated-Le Bas method at normal boiling point)

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³):
268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):

Entropy of Fusion, ∆S_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.122 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.81 × 10⁻³ (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00579, 0.00349 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_{L}/Pa) = −4382/(T/K) + 12.46 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
23.51 (calculated-QSAR-MCI χ, Sabljić & Güsten 1989)
18.48 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{ow}:
5.86 (calculated-TSA, Burkhard 1984)
6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0161 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{oa}:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{b}:

Sorption Partition Coefficient, log K_{OC}:
5.66 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, t\textsubscript{1/2}:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k\textsubscript{OH} for reaction with OH radical, k\textsubscript{NO3} with NO\textsubscript{3} radical and k\textsubscript{O3} with O\textsubscript{3} as indicated, *data at other temperatures see reference:
k\textsubscript{OH}(calc) = (0.4–0.9) $\times$ 10\textsuperscript{-12} cm\textsuperscript{3} molecule\textsuperscript{-1} s\textsuperscript{-1} for tetrachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k\textsubscript{OH}(calc) = (0.36–1.7) $\times$ 10\textsuperscript{-12} cm\textsuperscript{3} molecule\textsuperscript{-1} s\textsuperscript{-1} for tetrachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k\textsubscript{1} and k\textsubscript{2}):
k\textsubscript{2} = 0.008 d\textsuperscript{-1} with t\textsubscript{1/2} = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k\textsubscript{2} = 0.004 d\textsuperscript{-1} with t\textsubscript{1/2} = 157 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration t\textsubscript{1/2} = 91 d for high-dose treatment, t\textsubscript{1/2} = 157 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.56 2,3,3′,4′-Tetrachlorobiphenyl (PCB-56)

Common Name: 2,3,3′,4′-Tetrachlorobiphenyl
Synonym: PCB-56, 2,3,3′,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′-tetrachlorobiphenyl
CAS Registry No: 41464-41-9
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C): 95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0389 (20°C, supercooled liquid, Murphy et al. 1987)
0.0989 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.0146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0115 (calculated-QSAR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.96 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00434, 0.00327 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.17 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
0.00331, 0.00468 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4382/(T/K) + 12.33 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
9.45 (calculated-P/C, Burkhard 1984)
16.41 (20°C, calculated-P/C, Murphy et al. 1987)
13.27 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
15.34 (calculated-QSAR, Dunnivant et al. 1992)
8.24 (calculated-QSAR, Achman et al. 1993)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
27.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 32 ± 3 kJ/mol, ΔS_{fus} = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
5.85 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
6.11 (calculated, Miertus & Jakus 1990)
5.85 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$:
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
5.66 (suspended particulate matter, Burkhard 1984)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{\frac{1}{2}}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(aq.) = 5.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{\frac{1}{2}} \sim 4–11 \text{ d}$ in freshwater systems, $t_{\frac{1}{2}} = 0.1–10 \text{ d}$ in cloud water, $t_{\frac{1}{2}} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota:
7.1.1.57 2,3,3′,5-Tetrachlorobiphenyl (PCB-57)

Common Name: 2,3,3′,5-Tetrachlorobiphenyl
Synonym: PCB-57
Chemical Name: 2,3,3′,5-tetrachlorobiphenyl
CAS Registry No: 70424-87-8
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 291.988

Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$

Water Solubility (g/m³ or mg/L at 25°C):
0.106 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0718 (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00767 (GC-RI correlation, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
19.76 (calculated-P/C, Burkhard 1984)
37.59 (calculated-QSAR-MCl $\chi$, Sabljic & Güsten 1989)
27.40 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R$; $R$ is the ideal gas constant, $\Delta H_{\text{fus}} = 28 \pm 3$ kJ/mol, $\Delta S_{\text{fus}} = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
5.91 (calculated, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.1376 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{\text{oa}}$:
8.69 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{\text{oc}}$:
5.71 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constant and Half-Lives:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36-1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.58 2,3,3',5'-Tetrachlorobiphenyl (PCB-58)

Common Name: 2,3,3',5'-Tetrachlorobiphenyl
Synonym: PCB-58
Chemical Name: 2,3,3',5'-tetrachlorobiphenyl
CAS Registry No: 41464-43-1
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.106 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00558 (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C):
9.62 × 10⁻⁴ (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.80 – 5600/(T/K) (GC-RT correlation, Tateya et al. 1988)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
16.11 (calculated-P/C, Burkhard 1984)
45.46 (calculated-QSAR-MCI χ, Sabljić & Güsten 1989)
25.33 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\ln K_{AW} = -\Delta H_{fus}/RT + \Delta S_{fus}/R; R is the ideal gas constant, \Delta H_{fus} = 28 ± 3 kJ/mol, \Delta S_{fus} = 0.06 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
5.91 (calculated-TSA, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a)
6.17 (recommended, Hansch et al. 1995)
6.0904 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
8.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
5.71 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

Volatileization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:

\[
k_{\text{OH}}(\text{calc}) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 25–60 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}
\]

\[
k_{\text{OH}}(\text{calc}) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 8.5–40 \text{ d at room temp. (Kwok et al. 1995)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.59 2,3,3′,6-Tetrachlorobiphenyl (PCB-59)

Common Name: 2,3,3′,6-Tetrachlorobiphenyl
Synonym: PCB-59
Chemical Name: 2,3,3′,6-tetrachlorobiphenyl
CAS Registry No: 74472-33-6
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.131 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00733 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
0.0155 (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0164 (GC-RJ correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
34.65 (calculated-P/C, Burkhard 1984)
36.58 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.81 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 27 ± 2 kJ/mol, ΔS_{fus} = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated, Burkhard 1984)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8476 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{BC}:
Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 132 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 135 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:

Biota: depuration $t_{1/2} = 132$ d for high-dose treatment, $t_{1/2} = 135$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs) 1651

7.1.1.60 2,3,4,4′-Tetrachlorobiphenyl (PCB-60)

Common Name: 2,3,4,4′-Tetrachlorobiphenyl
Synonym: PCB-60, 2,3,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′-tetrachlorobiphenyl
CAS Registry No: 33025-41-1
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C):
- 128 (Weast 1972–73; Ruelle & Kesselring 1997)
- 142 (Saeki et al. 1971; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2024
Molar Volume (cm³/mol):
- 268.2 (calculated-Le Bas method at normal boiling point)
- 211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.0695 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.0168 (calculated-TSA, Mackay et al. 1980)
- 0.121 (calculated-TSA, supercooled liquid S_{L}, Burkhard et al. 1985b)
- 0.0389 (20°C, supercooled liquid S_{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.0902, 0.0485, 0.0254, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.0359, 0.0273 (Nirmalakhandan & Speece 1989)
- 0.0146 (calculated-TSA, Abramowitz & Yalkowsky 1990)
- 0.045 (calculated-MCI χ, Patil 1991)
- 0.00274 (calculated-QSPR, Dunnivant et al. 1992)
- 0.0067, 0.0176 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.000319 (GC-RI correlation, Burkhard et al. 1985a)
- 0.00427 (supercooled liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)
- 0.00527, 0.00414 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.00217 (20°C, supercooled liquid P_{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4660/(T/K) (GC-RT correlation, Tateya et al. 1988)
- 0.00331, 0.00458 (supercooled liquid P_{L}: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = – 4282/(T/K) + 12.42 (supercooled liquid P_{L}, GC-RT correlation, Falconer Bidleman 1994)
- 0.0157 (supercooled liquid P_{L}, calculated-MCI 3χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C):
- 84.20 (batch stripping, Atlas et al. 1982)
- 10.34 (calculated-P/C, Burkhard et al. 1985b)
- 16.41 (20°C, calculated-P/C, Murphy et al. 1987)
15.40 \text{(calculated-QSAR-MCI } \chi, \text{ Sabljic & Güsten 1989)}

15.48 \text{(calculated-QSPR, Dunnivant et al. 1992)}

35.1 \text{(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)}

\ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; \text{ R is the ideal gas constant, } \Delta H_{f} = 28 \pm 3 \text{ kJ/mol, } \Delta S_{f} = 0.06 \pm 0.01 \text{ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004)}

Octanol/Water Partition Coefficient, log $K_{ow}$:

5.87 \text{(calculated-TSA, Burkhard 1984)}

5.84 \text{(HPLC-RT correlation calculated-}\pi, \text{ Rapaport & Eisenreich 1984)}

5.90 \text{(selected, Shiui & Mackay 1986)}

5.89, 6.15, 6.57, 6.37 \text{(RP-HPLC-}K' \text{ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)}

6.11 \text{(calculated-TSA, Hawker & Connell 1988a)}

5.88 \text{(calculated-MCI } \chi, \text{ Patil 1991)}

7.8733 \text{(calculated-UNIFAC group contribution, Chen et al. 1993)}

6.01 \text{(recommended, Sangster 1993)}

5.84 \text{(quoted, Hansch et al. 1995)}

5.95, 5.33–6.24 \text{(calculated-Characteristic Root Index CRI, minimum-maximum range, Saçan & Inel 1995)}

6.0108 \text{(calculated-molecular properties MNDO-AM1 method, Makino 1998)}

Octanol/Air Partition Coefficient, log $K_{oa}$:

9.82 \text{(10°C, estimated, Thomas et al. 1998)}

9.21 \text{(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)}

Bioconcentration Factor, log $BCF$:

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$

6.20, 5.0 \text{(Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)}

Sorption Partition Coefficient, log $K_{oc}$:

5.67 \text{(suspected particulate matter, calculated-$K_{ow}$, Burkhard 1984)}

6.10 \text{(organic carbon, obs., Murray & Andren 1992)}

5.03 \text{(soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)}

5.30 \text{(soil, calculated-$K_{ow}$, Girvin & Scott 1997)}

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volutilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.4 \times 10^{9} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} = 4–11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1–10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 10 \text{ (food lipid mg)/(g worm lipid-d); } k_2 = 0.10 \text{ d}^{-1} \text{ (earthworm, Wågman et al. 2001)}$
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \approx 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 7$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.61 2,3,4,5-Tetrachlorobiphenyl (PCB-61)

Common Name: 2,3,4,5-Tetrachlorobiphenyl
Synonym: PCB-61, 2,3,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5-tetrachlorobiphenyl
CAS Registry No: 33284-53-6
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988

Melting Point (°C):
92.2  
(Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C): 1.2024

Molar Volume (cm³/mol):
268.2  
(calculated-Le Bas method at normal boiling point)
211.6  
(Ruelle & Kesselring 1997)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
25.2  
(differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
69.45  
(Miller et al. 1984)
69.25, 64.3  
(exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
0.217  
(Mackay et al. 1980)
0.218  
(Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0192  
(generator column-GC/ECD, Weil et al. 1974)
0.0209  
(shake flask-GC/ECD, Haque & Schmedding 1975)
0.0099  
(generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.0209  
(generator column-GC/ECD, Miller et al. 1984, 1985)
0.0207, 0.030, 0.0180, 0.0243  
(RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.014  
(generator column-GC, Dunnivant & Elzerman 1988)
0.0137  
(generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
0.0136  
(shake flask-GC/ECD, Li & Andren 1994)
0.0156* ± 0.0004  
(generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)

ln $x = -3.967 - 4970.5/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0624  
(calculated-mp and $K_{\text{ow}}$, Ran et al. 2002)
0.106, 0.101  
(supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_l/(mol m⁻³)] = –839/(T/K) – 0.626  
(supercooled liquid, linear regression of literature data, Li et al. 2003)
log [S_l/(mol m⁻³)] = –1043/(T/K) + 0.037  
(supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0013  
(GC-RT correlation, Burkhard et al. 1985a)
0.00558  
(supercooled liquid P_t, GC-RI correlation, Burkhard et al. 1985b)
log (P_t/Pa) = -4382/(T/K) + 12.78  
(supercooled liquid P_t, GC-RT correlation, Falconer & Bidleman 1994)
1.854 × 10^{-8}  
(20°C, gas saturation-GC/ECD, measured range –20 to 20°C, Wania et al. 1994)
log (P_t/Pa) = 12.10 – 4632/(T/K); temp range –20 to +20°C (gas saturation-GC, Wania et al. 1994)
Polychlorinated Biphenyls (PCBs)

0.0144 (supercooled liq. P_L, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
0.00724, 0.00692 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)

log (P_L/P_a) = –4330/(T/K) + 12.38 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log (P_L/P_a) = –4193/(T/K) + 11.91 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
11.45 (calculated-P/C, Burkhard et al. 1985b)
17.53 (calculated-QSPR-MCI χ, Sabljic & Gusten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

ln K_{AW} = –ΔH_f/RT + ΔS_f/R; R is the ideal gas constant, ΔH_f = 28 ± 3 kJ/mol, ΔS_f = 0.06 ± 0.01 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

5.78 (HPLC-RT correlation, Sugiura et al. 1979)
5.90 (shake flask-GC, Platford 1982)
6.39 (RP-TLC-k’ correlation, Bruggeman et al. 1982)
6.74 (calculated-fragment const., Yalkowsky et al. 1983)
5.81 (calculated-TSA, Burkhard 1984)
5.72 (generator column-GC/EC, Miller et al. 1984, 1985)
5.90 (selected, Shiu & Mackay 1986)
6.38, 6.31, 6.57, 6.37 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.18, 6.04 (generator column-GC/EC; calculated-TSA, Hawker & Connell 1988a)
5.92, 6.74 (calculated-solvatochromic parameters and V_π, calculated-fragment additivity., Kamlet et al. 1988)
6.88, 6.74, 5.89, 6.04, 6.02 (calculated-π const., f const., MW, MCI χ, TSA, Doucette & Andre 1988)
3.69 (calculated-π const., De Bruijn et al. 1989)
6.406 ± 0.069 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.89 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
6.34 (generator column-GC, Li & Doucette 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.44 (recommended, Sangster 1993)
6.41 (recommended, Hansch et al. 1995)
5.97, 5.72–6.74 (calculated-Characteristic Root Index CRI; minimum-maximum range, Saçan & Inel 1995)
6.1472 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.00 (calculated-QSPR, Yeh & Hong 2002)
6.51 (calculated-CLOGP ver. 4, Ran et al. 2002)
6.17, 6.11 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
8.901* (20°C, generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
log K_{OA} = –2.90 + 3464/(T/K); temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
8.90 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = –2.89 + 3464.1/(T/K); temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.38–9.65 (10°C, estimated, Thomas et al. 1998)
10.19, 8.93; 8.90 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
8.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.80; 8.75 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.64, 8.55 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4660/(T/K) – 7.08 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
4.29, 3.57, 3.94, 3.90 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
Sorption Partition Coefficient, log $K_{OC}$:
- 5.61 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 4.93 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  $k_{OH}\text{(calc)} = (0.4–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau\text{(calc)} = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  $k_{OH}\text{(calc)} = (0.36–1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau\text{(calc)} = 8.5–40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 0.038$ d$^{-1}$ (golden orfe, Sugiura et al. 1979)
- $k_2 = 0.0022$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: $t_{1/2} = 312$ d in rainbow trout, and $t_{1/2} = 93$ d in its muscle 93 d (Niimi & Oliver 1983)

### TABLE 7.1.1.61.1

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aqueous solubility</strong></td>
<td><strong>Vapor pressure</strong></td>
<td><strong>log $K_{OA}$</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC/ECD</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^3$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>0.0056</td>
<td>$-20$</td>
</tr>
<tr>
<td>15</td>
<td>0.0102</td>
<td>$-10$</td>
</tr>
<tr>
<td>25</td>
<td>0.0156</td>
<td>0</td>
</tr>
<tr>
<td>35</td>
<td>0.0285</td>
<td>10</td>
</tr>
<tr>
<td>45</td>
<td>0.0560</td>
<td>20</td>
</tr>
</tbody>
</table>

$\Delta H_{subl/(kJ mol^{-1})} = 88.7$

for 5–45°C

$\Delta H_{sol/(kJ mol^{-1})}$ = 41.3

$\Delta H_{sol/(kJ mol^{-1})} = 66.3$

$\log (P/Pa) = A - B/(T/K)$

$A = 12.10$

$B = 4632$

temp range $-20$ to $20°C$

$\Delta H_{subl/(kJ mol^{-1})} = 88.7$

$\Delta H_{sol/(kJ mol^{-1})}$ = 41.3

$\log K_{OA} = A + B/T$

$A = -2.9$

$B = 3464.1$
FIGURE 7.1.1.61.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 2,3,4,5-tetrachlorobiphenyl (PCB-61).
Common Name: 2,3,4,6-Tetrachlorobiphenyl
Synonym: PCB-62
Chemical Name: 2,3,4,6-tetrachlorobiphenyl
CAS Registry No: 54230-23-7
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C): 77 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0463 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
0.0158 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0167 (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
30.70 (calculated-P/C, Burkhard 1984)
37.08 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC, Brunner et al. 1990)
37.47 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 27 ± 2 kJ/mol, ΔS_{fus} = 0.05 ± 0.01 kJ/mol K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
5.79 (calculated, Burkhard 1984)
5.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0323 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{OC}:
5.59 (suspended particulate matter, Burkhard 1984)
Polychlorinated Biphenyls (PCBs)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volutilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
Common Name: 2,3,4′,5-Tetrachlorobiphenyl
Synonym: PCB-63, 2,3,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,5-tetrachlorobiphenyl
CAS Registry No: 74472-34-7
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988

Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)

Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.105 (S, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0263 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00727 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.36 × 10^{-3} (P, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681 (GC-R1 correlation, Burkhard et al. 1985b)
2.64 × 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00724 (supercooled liquid P, GC-R1 correlation, Fischer et al. 1992)
$\log(P_{s}/P_{a}) = -4382/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
17.73 (calculated-P/C, Burkhard 1984)
29.28 (20°C, calculated-P/C, Murphy et al. 1987)
29.60 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
8.24 (calculated-QSAR, Achman et al. 1993)
25.59 (calculated-QSPR, Dunnivant et al. 1992)
24.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{\text{AW}} = -\Delta H_{\text{aw}}/RT + \Delta S_{\text{aw}}/R$; R is the ideal gas constant, $\Delta H_{\text{aw}} = 25 \pm 2$ kJ/mol, $\Delta S_{\text{aw}} = 0.05 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
5.91 (calculated-TSA, Burkhard 1984)
6.10 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.10 (recommended, Sangster 1993)
6.1262 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:
- 10.15, 9.06 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):

Sorption Partition Coefficient, \( \log K_{OC} \):
- 5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatile:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated; *data at other temperatures see reference:
- \( k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12} \, \text{cm}^3 \, \text{molecule}^{-1} \, \text{s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 25–60 \, \text{d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
- \( k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12} \, \text{cm}^3 \, \text{molecule}^{-1} \, \text{s}^{-1} \) for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 8.5–40 \, \text{d} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
- \( k_2 = 0.003 \, \text{d}^{-1} \) with \( t_\frac{1}{2} = 219 \, \text{d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.004 \, \text{d}^{-1} \) with \( t_\frac{1}{2} = 172 \, \text{d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration \( t_\frac{1}{2} = 219 \, \text{d} \) for high-dose treatment, \( t_\frac{1}{2} = 172 \, \text{d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.64 2,3,4′,6-Tetrachlorobiphenyl (PCB-64)

Common Name: 2,3,4′,6-Tetrachlorobiphenyl
Synonym: PCB-64, 2,3,4′,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,6-tetrachlorobiphenyl
CAS Registry No: 52663-58-8
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988
Melting Point (°C):
57 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.130 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0937 (20°C, supercooled liquid, Murphy et al. 1987)
0.028 (RP-HPLC-k′ correlation, Brodsky & Ballischmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0138 (P_l supercooled liquid, GC-RT correlation Burkhard et al. 1985a)
0.0146 (GC-RI correlation, Burkhard et al. 1985b)
5.51 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.70 – 4510/(T/K) (GC-RT correlation, Tateya et al. 1988)
log (P/P_l) = –4229/(T/K) + 12.30 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
31.01 (calculated-P/C, Burkhard 1984)
17.25 (20°C, calculated-P/C, Murphy et al. 1987)
28.37 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.2 (wetted-wall column-GC, Brunner et al. 1990)
27.59 (calculated-QSPR, Dunnivant et al. 1992)
24.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.4 (from 11°C exp. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 24 ± 2 kJ/mol, ΔS_{fus} = 0.05 ± 0.01 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
5.84 (calculated-TSA, Burkhard 1984)
5.76 (RP-HPLC-k′ correlation, Brodsky & Ballischmiter 1988)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0 (calculated-TSA, Murray & Andren 1992)
5.76 (recommended, Sangster 1993)
5.8251 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log K\textsubscript{OA} at 25°C or as indicated and reported temperature dependence equations:

- 8.41; 7.91 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- \[ \log K\textsubscript{OA} = -6.43 + 4420/(T/K) \] (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.80 (quoted, Kömp & McLachlan 1997b)
- 9.62, 8.63; 8.74 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 8.54 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K\textsubscript{B}:

Sorption Partition Coefficient, log K\textsubscript{OC}:

- 5.64 (suspended particular matter, Burkhard 1984)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, t\textsubscript{1/2}:

Volatile Partitioning:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k\textsubscript{OH} for reaction with OH radical, k\textsubscript{NO3} with NO\textsubscript{3} radical and k\textsubscript{O3} with O\textsubscript{3} or as indicated, *data at other temperatures see reference:

\[ k\text{OH(calc)} = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau\text{(calc)} = 25 - 60 \text{ d, due to gas-phase loss process at room temp.} \) (Atkinson 1987)

\[ k\text{OH(calc)} = (0.36-1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau\text{(calc)} = 8.5-40 \text{ d at room temp.} \) (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k\textsubscript{1} and k\textsubscript{2}):

\[ k\textsubscript{2} = 0.005 \text{ d}^{-1} \text{ with } t\textsubscript{1/2} = 140 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)} \]

\[ k\textsubscript{2} = 0.004 \text{ d}^{-1} \text{ with } t\textsubscript{1/2} = 160 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)} \]

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration \( t\text{_{1/2}} = 140 \text{ d for high-dose treatment, } t\text{_{1/2}} = 160 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)} \)
7.1.1.65 2,3,5,6-Tetrachlorobiphenyl (PCB-65)

Common Name: 2,3,5,6-Tetrachlorobiphenyl
Synonym: PCB-65, 2,3,5,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,5,6-tetrachlorobiphenyl
CAS Registry No: 33284-54-7
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988

Melting Point (°C):
77–77.5 (Bolgar 1973)
79.0 (Burkhard 1984; Brodsky & Ballschmiter 1988)

Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.295 (mp at 79°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.162 (S_1, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0099, 0.0216, 0.0119, 0.0279 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0431 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0151 (P_1, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00467 (GC-RI correlation, Burkhard et al. 1985b)
0.0151 (supercooled liquid P_1, GC-RI correlation, Fischer et al. 1992)
log (P_1/P_a) = −4229/(T/K) + 12.33 (GC-RT correlation, supercooled liquid, Falcoker & Bidleman 1994)
0.0238 (P_1, calculated-MCI χ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry’s Law Constant (Pa·m³/mol at 25°C):
27.26 (calculated-P/C, Burkhard 1984)
31.01 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
34.10 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_{g}/RT + ΔS_{g}/R; R is the ideal gas constant, ΔH_{g} = 25 ± 2 kJ/mol, ΔS_{g} = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.77 (calculated-TSA, Burkhard 1984)
6.07, 5.95, 5.98, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.94; 5.86 (generator column-GC; calculated-TSA, Hawker & Connell 1988a)
5.96 (recommended, Sangster 1993)
7.8733 (calculated-UNIFAC group contribution method, Chen et al. 1993)
Polychlorinated Biphenyls (PCBs)

5.86 (recommended, Hansch et al. 1995)
5.81; 5.46–5.96 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.0133 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
5.83 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$:
8.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
2.46 ($P. reticulata$, Devillers et al. 1996)

Sorption Partition Coefficient, log $K_{OC}$:
5.57 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\lambda$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ as indicated, *data at other temperatures see reference:
$$k_{OH}(\text{calc}) = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$$k_{OH}(\text{calc}) = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.66 2,3′,4,4′-Tetrachlorobiphenyl (PCB-66)

Common Name: 2,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-66, 2,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-10-0
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988

Melting Point (°C):
- 124 (Saeki et al. 1971; Hutzinger et al. 1974)
- 127–127.5 (Webb & McCall 1972)

Boiling Point (°C): 
Density (g/cm³): 268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.105 (Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.0168 (calculated-TSA, Mackay et al. 1980)
- 0.098 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
- 0.00474 (calculated-fragment solubility constants, Wákitia et al. 1986)
- 0.0368 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.068 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
- 0.0273 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
- 0.0116 (calculated-TSA, Abramowitz & Yalkowsky 1990)
- 0.045 (calculated-MCI χ, Patil 1991)
- 0.00446 (calculated-QSPR, Dunnivant et al. 1992)
- 0.0216 (calculated-group contribution method, Kühne et al. 1995)
- 0.0266 (calculated-mp and K_{o/w}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.00616 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
- 0.000494 (GC-RI correlation, Burkhard et al. 1985a)
- 0.00459 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
- 0.00569, 0.00507 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.00252 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
- 0.00427, 0.0059 (supercooled liquid P_L; GC-RI correlation, different stationary phases, Fischer et al. 1992)
- log (P_L/Pa) = – 4349/(T/K) + 12.38 (GC-RT correlation, Falconer & Bidleman 1994)
- 0.00347 (supercooled liquid P_L, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
- 84.20 (calculated-P/C, Murphy et al. 1983)
- 13.68 (calculated-P/C, Burkhard et al. 1985b)
Polychlorinated Biphenyls (PCBs)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octanol/Water Partition Coefficient, log $K_{OW}$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.90</td>
<td>(HPLC-RT correlation, Shaw &amp; Connell 1982)</td>
<td></td>
</tr>
<tr>
<td>5.80, 6.31</td>
<td>(HPLC-RT correlation, Rapaport &amp; Eisenreich 1984)</td>
<td></td>
</tr>
<tr>
<td>5.98</td>
<td>(RP-HPLC-k′ correlation, Brodsky &amp; Ballschmiter 1988)</td>
<td></td>
</tr>
<tr>
<td>6.31</td>
<td>(generator column-GC/ECD, Hawker &amp; Connell 1988a)</td>
<td></td>
</tr>
<tr>
<td>6.09</td>
<td>(generator column-GC, Larsen et al. 1992)</td>
<td></td>
</tr>
<tr>
<td>6.12</td>
<td>(recommended, Sangster 1993)</td>
<td></td>
</tr>
<tr>
<td>6.31</td>
<td>(recommended, Hansch et al. 1995)</td>
<td></td>
</tr>
<tr>
<td>Octanol/Air Partition Coefficient, log $K_{OA}$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>log $K_{OA}$ = -3.82 + 3827/(T/K); temp range 0–30°C (generator column-GC, Harner &amp; Bidleman 1996)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.73</td>
<td>(10°C, estimated, Thomas et al. 1998)</td>
<td></td>
</tr>
<tr>
<td>10.33, 9.29; 9.22</td>
<td>(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)</td>
<td></td>
</tr>
<tr>
<td>9.36</td>
<td>(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)</td>
<td></td>
</tr>
<tr>
<td>Bioconcentration Factor, log $BCF$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.45</td>
<td>(worms, Oliver 1987c)</td>
<td></td>
</tr>
<tr>
<td>3.18–4.62</td>
<td>(various marine species, mean dry wt. BCF, Hope et al. 1998)</td>
<td></td>
</tr>
<tr>
<td>4.55–5.76</td>
<td>(various marine species, mean lipid-normalized BCF, Hope et al. 1998)</td>
<td></td>
</tr>
<tr>
<td>Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.80, 4.90</td>
<td>(Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)</td>
<td></td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log $K_{OC}$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.74</td>
<td>(suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)</td>
<td></td>
</tr>
<tr>
<td>4.72</td>
<td>(soil, calculated-S, Chou &amp; Griffin 1986)</td>
<td></td>
</tr>
<tr>
<td>5.23</td>
<td>(calculated after Karickhoff et al. 1979, Capel &amp; Eisenreich 1990)</td>
<td></td>
</tr>
<tr>
<td>4.90</td>
<td>(calculated after Schwarzbenbach &amp; Westall 1981, Capel &amp; Eisenreich 1990)</td>
<td></td>
</tr>
<tr>
<td>6.10</td>
<td>(organic carbon, obs., Murray &amp; Andren 1992)</td>
<td></td>
</tr>
<tr>
<td>4.90</td>
<td>(soil, calculated-QSPR Characteristic Root Index [CRI], Saçan &amp; Balcioglu 1996)</td>
<td></td>
</tr>
<tr>
<td>5.20</td>
<td>(soil, calculated-$K_{OW}$, Girvin &amp; Scott 1997)</td>
<td></td>
</tr>
<tr>
<td>Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Volatilization:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrolysis:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Photolysis:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxidation:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>rate constant $k$, for gas-phase second order reaction constants, $k_{OH}$, for reaction with OH radical, $k_{NO3}$, with NO$<em>3$ radical and $k</em>{O3}$ with O$<em>3$ or as indicated, *data at other temperatures see reference: $k</em>{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**k_{OH}(aq.) = 5.1 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from t_{1/2} \sim 4–11 d in freshwater systems, t_{1/2} = 0.1–10 d in cloud water, t_{1/2} > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)**

k_{OH(calc)} = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime \( \tau_{(calc)} = 8.5–40 \text{ d} \text{ at room temp.} \) (Kwok et al. 1995)

**Biodegradation:**

**Biotransformation:**

**Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:**

- \( \text{t}_{1/2} = 0.001 \text{ d}^{-1} \) (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)
- \( \text{t}_{1/2} = 0.009 \text{ d}^{-1} \text{ with t}_{1/2} = 82 \text{ d} \text{ and k}_2 = 0.013 \text{ d}^{-1} \text{ with t}_{1/2} = 55 \text{ d} \) for food concn of 21 ng/g and 158 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- \( \text{t}_{1/2} = 0.004 \text{ d}^{-1} \text{ with t}_{1/2} = 164 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- \( \text{t}_{1/2} = 0.003 \text{ d}^{-1} \text{ with t}_{1/2} = 225 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

**Half-Lives in the Environment:**

**Air:** calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

**Surface water:** half-lives range from \( \text{t}_{1/2} \sim 4–11 \text{ d} \) in freshwater systems, \( \text{t}_{1/2} = 0.1–10 \text{ d} \) in cloud water, \( \text{t}_{1/2} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991); photodegradation \( \text{t}_{1/2} = (7.1 ± 1.5) \text{ h} \) in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

**Groundwater:**

**Sediment:**

**Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are:**

\[ k = 0.067 \text{ d}^{-1} \text{ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, } k = 0.75 \text{ d}^{-1} \text{ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, } k = 1.18 \text{ d}^{-1} \text{ from Tarehee surface soil consist of sand and silt with 0.02% OC and } k = 0.32 \text{ d}^{-1} \text{ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are:**

\[ k = 0.00081 \text{ d}^{-1} \text{ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, } k = 0.0024 \text{ d}^{-1} \text{ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, } k = 0.00443 \text{ d}^{-1} \text{ from Tarehee surface soil consist of sand and silt with 0.02% OC and } k = 0.000295 \text{ d}^{-1} \text{ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).}

**Biota:** \( \text{t}_{1/2} = 670 \text{ d} \text{ in rainbow trout, and } \text{t}_{1/2} = 108 \text{ d} \text{ its muscle (Niimi & Oliver 1983)} \)

- \( \text{t}_{1/2} = 33 \text{ d in worms at 8°C(Oliver 1987c)} \)
- \( \text{depuration } \text{t}_{1/2} = 55–82 \text{ d} \text{ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)} \)
- \( \text{depuration } \text{t}_{1/2} = 164 \text{ d} \text{ for high-dose treatment, } \text{t}_{1/2} = 225 \text{ d} \text{ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)} \)
### TABLE 7.1.1.66.1
Reported Henry’s law constants and octanol-air partition coefficients of 2,3′,4,4′-tetrachlorobiphenyl (PCB-66) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log K&lt;sub&gt;OA&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bamford et al. 2000</strong></td>
<td><strong>Harner &amp; Bidleman 1996</strong></td>
</tr>
<tr>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m&lt;sup&gt;3&lt;/sup&gt;/mol)</td>
</tr>
<tr>
<td>4</td>
<td>14.17</td>
</tr>
<tr>
<td>11</td>
<td>19.80</td>
</tr>
<tr>
<td>18</td>
<td>27.25</td>
</tr>
<tr>
<td>25</td>
<td>36.97</td>
</tr>
<tr>
<td>31</td>
<td>47.51</td>
</tr>
</tbody>
</table>

\[
\ln K_{SW} = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}
\]

\[
K_{AW} \log K_{OA} = A + B/T
\]

- **enthalpy, entropy change:**
  - \(\Delta H/(kJ \cdot mol^{-1}) = 29.0 \pm 2.6\)
  - \(\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 62 \pm 8\)

### FIGURE 7.1.1.66.1
Logarithm of Henry’s law constant and K<sub>OA</sub> versus reciprocal temperature for 2,3′,4,4′-tetrachlorobiphenyl (PCB-66).
7.1.1.67  2,3’,4,5-Tetrachlorobiphenyl (PCB-67)

Common Name: 2,3’,4,5-Tetrachlorobiphenyl
Synonym: PCB-67, 2,3’,4,5-tetrachloro-1,1’-biphenyl
Chemical Name: 2,3’,4,5-tetrachlorobiphenyl
CAS Registry No: 73575-53-8
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C): 83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³): 268.2 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
\( 0.0987 \) (Sₜ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
\( 0.0351, 0.0298, 0.00804, 0.0266 \) (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
\( 0.0184 \) (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\( 0.00654 \) (Pₜ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
\( 0.0070 \) (GC-RI correlation, Burkhard et al. 1985b)
\( \log(P/\text{mmHg}) = 10.70 - 4530/(T/K) \) (GC-RT correlation, Tateya et al. 1988)
\( 0.00708 \) (supercooled liquid Pₜ, GC-RI correlation, Fischer et al. 1992)
\( \log(P/P_{\text{L}}) = -4382/(T/K) + 12.52 \), (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
\( 19.35 \) (calculated-P/C, Burkhard 1984)
\( 29.18 \) (calculated-QSAR-MCI \( \chi \), Sabljic & Güsten 1989)
\( 10.13 \) (wetted-wall column-GC/ECD, Brunner et al. 1990)
\( 23.70 \) (calculated-QSPR, Dunning et al. 1992)
\( 35.1 \) (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\( \ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R \); R is the ideal gas constant, \( \Delta H_{\text{fus}} = 28 \pm 3 \) kJ/mol, \( \Delta S_{\text{fus}} = 0.06 \pm 0.01 \) kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
\( 5.93 \) (calculated-TSA, Burkhard 1984)
\( 6.22, 6.32, 6.40, 6.33 \) (RP-HPLC-k’ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
\( 6.20 \) (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
\( 6.32 \) (recommended, Sangster 1993)
\( 6.2276 \) (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
9.06 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
5.73 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.68 2,3′,4,5′-Tetrachlorobiphenyl (PCB-68)

Common Name: 2,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-68
Chemical Name: 2,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 73575-52-7
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C):
71 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.085 (S₇ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
0.00679 (P₇ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00726 (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
23.30 (calculated-P/C, Burkhard 1984)
55.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.17 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₘw = –ΔH/RT + ΔS/R; R is the ideal gas constant, ΔH_f = 28 ± 3 kJ/mol, ΔS_f = 0.06 ± 0.01 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₘw:
5.99 (calculated-TSA, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2624 (calculated molecular properties MNDO-AM method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₘa:
8.66 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₛ:
5.79 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:

- $k_{OH}(calc) = (0.4–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

- $k_{OH}(calc) = (0.36–1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1 = 11$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.08$ d$^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 8$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.69 2,3′,4,6-Tetrachlorobiphenyl (PCB-69)

![Chemical Structure](image)

Common Name: 2,3′,4,6-Tetrachlorobiphenyl
Synonym: PCB-69
Chemical Name: 2,3′,4,6-tetrachlorobiphenyl
CAS Registry No: 60233-24-1
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C): 45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.105 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0097, 0.0146, 0.0184, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0169 (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0179, (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.60 – 4440/T (GC-RT correlation, Tateya et al. 1988)
0.01911 (supercooled liquid P_l, GC-RI correlation, Fischer et al. 1992)
log (P_l/Pa) = –4229/(T/K) + 12.43 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
47.12 (calculated-P/C, Burkhard 1984)
63.53 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
51.22 (calculated-QSAR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 27 ± 2 kJ/mol, ΔS_{fus} = 0.05 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
5.91 (calculated-TSA, Burkhard 1984)
6.09,6.06, 6.09, 5.89 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0068 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
8.47 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_b:

Sorption Partition Coefficient, log K_OC:
5.71 (suspended particulate matter, Burkhard et al. 1984)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

Volatile:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference: 
k_{OH(calc)} = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 25–60 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}
k_{OH(calc)} = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 8.5–40 \text{ d at room temp. (Kwok et al. 1995)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.70 2,3',4',5-Tetrachlorobiphenyl (PCB-70)

Common Name: 2,3',4',5-Tetrachlorobiphenyl  
Synonym: PCB-70, 2,3',4',5-tetrachloro-1,1'-biphenyl  
Chemical Name: 2,3',4',5-tetrachlorobiphenyl  
CAS Registry No: 32598-11-1  
Molecular Formula: C_{12}H_6Cl_4  
Molecular Weight: 291.988  
Melting Point (°C):  
  104 (Bellavita 1935; Hutzinger et al. 1974)  
  104–107 (Wallnöfer et al. 1973, Bolgar 1973)  
Boiling Point (°C):  

Density (g/cm³ at 20°C): 1.2024  
Molar Volume (cm³/mol):  
  268.2 (calculated-Le Bas method at normal boiling point)  
  211.6 (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ∆H_fus (kJ/mol):  
Entropy of Fusion, ∆S_fus (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F: 0.168 (mp at 104°C)  

Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
  0.041 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)  
  0.029 (calculated-TSA, Mackay et al. 1980)  
  0.022 (generator column-GC, Bruggeman et al. 1981)  
  0.099 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)  
  0.0091 (generator column-GC/ECD, Opperhuizen et al. 1985)  
  0.0104 (calculated-fragment solubility constants, Wakita et al. 1986)  
  0.0362 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)  
  0.0254, 0.0368, 0.0432, 0.030 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
  0.0273 (calculated-MCI χ, Nirmalakhandan & Speece 1989)  
  0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)  
  0.045 (calculated-MCI χ, Patil 1991)  
  0.0111 (calculated-QSPR, Dunnivant et al. 1992)  
  0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
  0.0463 (calculated-mp and K_{mp}, Ran et al. 2002)  

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
  0.00544, 0.00642 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)  
  0.00769 (calculated S × HLC, Burkhard et al. 1985a)  
  0.00919 (GC-RI correlation, Burkhard et al. 1985a)  
  0.00519 (supercooled liquid P_L, calculated-GC-RI, Burkhard et al. 1985b)  
  0.00526, 0.00551 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
  0.0060 (selected P_L, supercooled liquid, Shiu & Mackay 1986)
Polychlorinated Biphenyls (PCBs)

0.00236 (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log (P_{\text{mmHg}}) = 10.90 - 4640/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00447, 0.0063 (supercooled liquid $P_L$, GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = - 4431/(T/K) + 12.60$ (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m$^3$/mol at 25°C or as indicated):

20.26  (calculated-P/C, Murphy et al. 1983)
15.30  (calculated-P/C, Burkhard et al. 1985b)
19.05  (20°C, calculated-P/C, Murphy et al. 1987)
19.15  (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
10.13  (wetted-wall column-GC, Brunner et al. 1990)
20.50  (calculated-QSAR, Dunnivant et al. 1992)
17.2   (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3   (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_f/RT + \Delta S_f/R$; $R$ is the ideal gas constant, $\Delta H_f = 29 \pm 3$ kJ/mol, $\Delta S_f = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{ow}$:

5.95   (shake flask-GC, Tulp & Hutzinger 1978)
5.95   (HPLC-$k'$ correlation, McDuffie 1981)
6.39   (RP-TLC-$k'$ correlation, Bruggeman et al. 1982)
6.30   (HPLC-RT correlation, Shaw & Connell 1982)
5.72, 6.23 (HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.18   (HPLC-RT correlation, Opperhuizen et al. 1985)
6.01, 6.24, 6.36, 6.29 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.99   (generator column-GC, Larsen et al. 1992)
5.99   (HPLC-$k'$ correlation, Neogrohati & Hammers 1992)
5.7833 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.23   (recommended, Sangster 1993)
6.23   (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:

10.29, 9.22; 9.29 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
8.92   (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$ at 25°C or as indicated:

6.15   (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
6.20   (goldfish, 3% lipid, calculated-$K_{ow}$, Bruggeman et al. 1981)
4.62, 5.11 (goldfish, exptrl., correlated, Mackay & Hughes 1984)
4.32, 5.50 (guppy, lipid phase, Opperhuizen et al. 1985)
4.92   (guppy, Gobas et al. 1987)
4.62, 4.32 (fish, calculated-$C_d/C_w$ or $k_d/k_{lw}$, Connell & Hawker 1988; Hawker 1990)
5.08; 6.61 (22°C, zebrafish: log $BCF_w$ wet wt basis; log $BCF_L$ lipid wt basis, Fox et al. 1994)
4.32, 5.62; 4.742, 4.257 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, $K_{ow}$, Lu et al. 1999)
5.08, 6.61 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$

5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
Sorption Partition Coefficient, $\log K_{OC}$:

- 5.02, 4.86, 4.85, 4.69 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
- 5.73 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.6–6.8, 6.3 (suspended sediment, average, Oliver 1987a)
- 4.81 (algae > 50 µm, Oliver 1987a)
- 4.76 (correlated literature values in soils, Sklarew & Girvin 1987)
- 6.04 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 6.0 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 4.84 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
- 5.02; 5.07 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 4.81 (soil, calculated-$S$, Chou & Griffin 1986)
- 5.30 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
- 8.6, 4.80 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

- Volatilization:
  - Photolysis:
    - Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3^-$ radical and $k_{O_3}$ with O$_3^-$ as or indicated, *data at other temperatures see reference:
      - $k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
      - $k_{OH}(aq.) = 5.5 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{\frac{1}{2}} \sim 4–11$ d in freshwater systems, 0.1–10 d in cloud water, $t_{\frac{1}{2}} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
      - $k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 420$ d$^{-1}$; $k_2 = 0.01$ d$^{-1}$ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986, Clark et al. 1990))
  - $k_1 = 0.01, 0.0104$ d$^{-1}$ (goldfish, exp., correlated, Mackay & Hughes 1984)
  - $k_1 = 380$ d$^{-1}$; $k_2 = 0.018$ d$^{-1}$ (guppy, Opperhuizen et al. 1985)
  - $k_1 = 17.5$ h$^{-1}$; $1/k_2 = 2400$ h (goldfish, quoted, Hawker & Connell 1985)
  - log $k_1 = 2.58, 2.62$ d$^{-1}$; log $1/k_2 = 1.74, 2.0$ d (fish, quoted, Connell & Hawker 1988)
  - log $k_2 = -2.0$ d$^{-1}$ (fish, quoted, Thomann 1989)
  - $k_1 = 3340$ d$^{-1}$; $k_2 = 0.0280$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
  - $k_1 = 0.00043$ h$^{-1}$; $k_2 = 0.170$ h$^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
  - $k_1 = 10$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.09$ d$^{-1}$ (earthworm, Wågman et al. 2001)
  - $k_1 = 0.004$ d$^{-1}$ with $t_{\frac{1}{2}} = 167$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.003$ d$^{-1}$ with $t_{\frac{1}{2}} = 217$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

- Half-Lives in the Environment:
  - Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
  - tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).
Polychlorinated Biphenyls (PCBs)

Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991); photodegradation $t_{1/2} = 4.87$ min when irradiated in a TiO$_2$ semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:

Sediment:

Soil:

Biota: clearance $t_{1/2} = 60$ d in goldfish (static equilibration system, 23-d exposure, Bruggeman et al. 1981) $t_{1/2} = 38.6$ d in guppy (Opperhuizen et al. 1985); elimination $t_{1/2} = 8$ d in earthworm given contaminated food (Wågman et al. 2001) depuration $t_{1/2} = 167$ d for high-dose treatment, $t_{1/2} = 217$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
### 7.1.1.71 2,3',4',6-Tetrachlorobiphenyl (PCB-71)

![Chemical structure of 2,3',4',6-Tetrachlorobiphenyl](image)

**Common Name:** 2,3',4',6-Tetrachlorobiphenyl  
**Synonym:** PCB-71  
**Chemical Name:** 2,3',4',6-tetrachlorobiphenyl  
**CAS Registry No:** 41464-46-4  
**Molecular Formula:** C₁₂H₆Cl₄  
**Molecular Weight:** 291.988  

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>57 (estimated, Abramowitz &amp; Yalkowsky 1990)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>268.2 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔH_fus (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ΔS_fus (J/mol K)</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F</td>
<td></td>
</tr>
</tbody>
</table>
| Water Solubility (g/m³ or mg/L at 25°C) | 0.123 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.0278 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)  
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
| Vapor Pressure (Pa at 25°C and reported temperature dependence equations) | 9.59 × 10⁻³ (P_l supercooled liquid, Burkhard et al. 1985a)  
0.0102 (GC-RI correlation, Burkhard et al. 1985b)  
0.00912, 0.00877 (supercooled liquid P_l, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
0.00776, 0.0115 (supercooled liquid P_l, GC-RI correlation, different stationary phases, Fischer et al. 1992)  
log (P_l/Pa) = −4229/(T/K) + 12.14 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
| Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated) | 22.80 (calculated-P/C, Burkhard 1984)  
32.53 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)  
14.31 (calculated-QSPR, Achman et al. 1993)  
31.82 (calculated-QSPR, Dunnivant et al. 1992)  
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
ln K_AW = −ΔH_fus/RT + ΔS_fus/R; R is the ideal gas constant, ΔH_fus = 27 ± 2 kJ/mol, ΔS_fus = 0.05 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004  
| Octanol/Water Partition Coefficient, log K_{ow} | 5.86 (calculated-TSA, Burkhard 1984)  
5.76 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)  
5.98 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)  
5.7206 (calculated-molecular properties MNDO-AM1 method, Makino 1998)  
| Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated | 9.78, 8.84; 8.98 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)  
8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)  

Polychlorinated Biphenyls (PCBs)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH(aq.)} = 5.7 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH(calc)} = (0.36 – 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota:
7.1.1.72 2,3',5,5'-Tetrachlorobiphenyl (PCB-72)

Common Name: 2,3',5,5'-Tetrachlorobiphenyl
Synonym: PCB-72
Chemical Name: 2,3',5,5'-tetrachlorobiphenyl
CAS Registry No: 41464-42-0
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C): 56 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Volatileization:**
**Photolysis:**
**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 – 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40 \text{ d}$ at room temp. (Kwok et al. 1995)

**Hydrolysis:**
**Biodegradation:**
**Biotransformation:**
**Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

**Half-Lives in the Environment:**
- **Air:** calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

**Surface water:**
**Ground water:**
**Sediment:**
**Soil:**
**Biota:**
7.1.1.73 2,3′,5′,6-Tetrachlorobiphenyl (PCB-73)

Common Name: 2,3′,5′,6-Tetrachlorobiphenyl
Synonym: PCB-73
Chemical Name: 2,3′,5′,6-tetrachlorobiphenyl
CAS Registry No: 74338-23-1
Molecular Formula: C_{12}H_{6}Cl_{4}
Molecular Weight: 291.988
Melting Point (°C):
66 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
268.2 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
0.0142 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.0150, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
38.91 (calculated-P/C, Burkhard 1984)
61.81 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
52.69 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = -ΔH_{g}/RT + ΔS_{g}/R; R is the ideal gas constant, ΔH_{g} = 27 ± 2 kJ/mol, ΔS_{g} = 0.05 ± 0.01 kJ/mol-K
(bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8026 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
7.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4 - 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25$–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36 - 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5$–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–0 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–0 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.74 2,4,4',5-Tetrachlorobiphenyl (PCB-74)

Common Name: 2,4,4’,5-Tetrachlorobiphenyl
Synonym: PCB-74, 2,4,4’,5-tetrachloro-1,1’-biphenyl
Chemical Name: 2,4,4’,5-tetrachlorobiphenyl
CAS Registry No: 32690-93-0
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C): 125 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F:
0.102 (calcd-assuming ΔS_fus = 56 J/mol K, Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0978 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0306 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.0116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00453 (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0058 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00209, 0.000636, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00731, 0.00769 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.12 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.80 – 4600/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00479, 0.00631 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (PL/Pa) = –4382/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0116 (P_L, calculated-MCI 3 χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
17.33 (calculated-P/C, Burkhard 1984)
21.18 (20°C,calculated-P/C, Murphy et al. 1987)
21.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
21.76 (calculated-QSPR, Dunnivant et al. 1992)
23.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.2 (from 11°C exp. data and compensation point, Bamford et al. 2002)
\( \ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R; \) R is the ideal gas constant, \( \Delta H_H = 25 \pm 2 \text{ kJ/mol}, \Delta S_H = 0.05 \pm 0.01 \text{ kJ/mol·K} \) (Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 6.16, 6.67 (HPLC-k’ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 6.10 (RP-HPLC-k’ correlation, Brodsky & Ballischminter 1988)
- 6.10 (recommended, Sangster 1993)
- 6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 10.25, 9.14; 8.96 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 9.38–9.65 (10°C, estimated, Thomas et al. 1998)
- 9.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Biota Sediment Accumulation Factor, BSAF:
- 51 (trout in Lake Ontario, Niimi 1996)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
- 5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:
- 5.74 (suspended particulate matter, Burkhard 1984)
- 6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.0 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 5.50 (soil-organic carbon, calculated-$K_{OW}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Volutilization:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:
- $k_{OH}(calc) = (0.4 – 0.9) \times 10^{–12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}(aq.) = 5.4 \times 10^9$ dm$^3$ mol$^{-1}$ s$^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{½} \sim 4–11$ d in freshwater systems, $t_{½} = 0.1–10$ d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
- $k_{OH}(calc) = (0.36 – 1.7) \times 10^{–12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.004$ d$^{-1}$ with $t_{½} = 172$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.003$ d$^{-1}$ with $t_{½} = 220$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{1/2} \sim 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 172$ d for high-dose treatment, $t_{1/2} = 220$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.75 2,4,4′,6-Tetrachlorobiphenyl (PCB-75)

![Chemical Structure](image)

**Common Name:** 2,4,4′,6-Tetrachlorobiphenyl  
**Synonym:** PCB-75, 2,4,4′,6-tetrachloro-1,1′-biphenyl  
**Chemical Name:** 2,4,4′,6-tetrachlorobiphenyl  
**CAS Registry No:** 32598-12-2  
**Molecular Formula:** C₁₂H₆Cl₄  
**Molecular Weight:** 291.988  
**Melting Point (°C):** 93.0 (calculated, Abramowitz & Yalkowsky 1990)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 268.2 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)  
**Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):**  
**Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), \( F \):**  
**Water Solubility (g/m³ or mg/L at 25°C):**  
<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.104</td>
<td>(supercooled liquid ( S_L ), calculated-TSA, Burkhard et al. 1985b)</td>
<td></td>
</tr>
<tr>
<td>0.00967, 0.0127, 0.0122, 0.0180</td>
<td>(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
<td></td>
</tr>
<tr>
<td>0.091</td>
<td>(generator column-GC/ECD, Dunnivant &amp; Elzerman 1988)</td>
<td></td>
</tr>
<tr>
<td>0.0184</td>
<td>(calculated-TSA, Abramowitz &amp; Yalkowsky 1990)</td>
<td></td>
</tr>
<tr>
<td>0.045</td>
<td>(calculated-MCI ( \chi ), Patil 1991)</td>
<td></td>
</tr>
<tr>
<td>0.0804</td>
<td>(calculated-mp and K(_{\text{OW}}), Ran et al. 2002)</td>
<td></td>
</tr>
</tbody>
</table>

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0204, 0.0158, 0.00419</td>
<td>(calculated-MW, GC-RI correlation, calculated-MCI ( \chi ), Burkhard et al. 1985a)</td>
<td></td>
</tr>
<tr>
<td>0.0150</td>
<td>(supercooled liquid ( P_L ), GC-RI correlation, Burkhard et al. 1985b)</td>
<td></td>
</tr>
<tr>
<td>0.0179, 0.0202</td>
<td>(supercooled liquid ( P_L ), GC-RT correlation, different stationary phases, Foreman &amp; Bidleman 1985)</td>
<td></td>
</tr>
</tbody>
</table>

\[
\log (P_L/Pa) = \frac{-4229/(T/K) + 12.44}{(GC-RT correlation, Falconer & Bidleman 1994)}
\]

**Henry’s Law Constant (Pa m³/mol at 25°C):**  
<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>42.25</td>
<td>(calculated-P/C, Burkhard et al. 1985b)</td>
<td></td>
</tr>
<tr>
<td>42.25</td>
<td>(batch stripping, Dunnivant &amp; Elzerman 1988)</td>
<td></td>
</tr>
<tr>
<td>55.32</td>
<td>(calculated- QSPR-MCI ( \chi ), Sabljic &amp; Güsten 1989)</td>
<td></td>
</tr>
<tr>
<td>47.07</td>
<td>(calculated-QSPR, Dunnivant et al. 1992)</td>
<td></td>
</tr>
<tr>
<td>35.0</td>
<td>(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)</td>
<td></td>
</tr>
</tbody>
</table>

\[
\ln K_{\text{AW}} = -\frac{\Delta H_{\text{fus}}}{RT} + \frac{\Delta S_{\text{fus}}}{R}; \text{ R is the ideal gas constant, } \Delta H_{\text{fus}} = 27 \pm 2 \text{ kJ/mol, } \Delta S_{\text{fus}} = 0.05 \pm 0.01 \text{ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004}}
\]

**Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):**  
<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.08, 6.10, 5.97, 5.97</td>
<td>(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmiter 1988)</td>
<td></td>
</tr>
<tr>
<td>6.03</td>
<td>(recommended, Sangster 1993)</td>
<td></td>
</tr>
</tbody>
</table>
Octanol/Air Partition Coefficient, log $K_{OA}$:

8.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

5.72 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volutilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 – 1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:
7.1.1.76 2,3’,4’,5’-Tetrachlorobiphenyl (PCB-76)

Common Name: 2,3’,4’,5’-Tetrachlorobiphenyl
Synonym: PCB-76, 2,3’,4’,5’-tetrachlorobiphenyl
Chemical Name: 2,3’,4’,5’-tetrachlorobiphenyl
CAS Registry No: 70362-48-0
Molecular Formula: C\textsubscript{12}H\textsubscript{6}Cl\textsubscript{4}
Molecular Weight: 291.988
Melting Point (°C): 89 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆\textsubscript{Hfus} (kJ/mol):
Entropy of Fusion, ∆\textsubscript{Sfus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆\textsubscript{Sfus} = 56 J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
0.114 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0551 (20°C, supercooled liquid, Murphy et al. 1987)
0.0569 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0150 (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00512, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00602, 0.00426 (supercooled liquid P\textsubscript{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.44 × 10\textsuperscript{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00447, 0.00646 (supercooled liquid P\textsubscript{L}; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P\textsubscript{L}/Pa) = –4382/(T/K) + 12.48 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C or as indicated):
12.16 (calculated-P/C, Burkhard 1984)
12.97 (20°C, calculated-P/C, Murphy et al. 1987)
22.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.13 (calculated-QSPR, Achman et al. 1993)
24.19 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K\textsubscript{AW} = −\Delta H\textsubscript{f}/RT + \Delta S\textsubscript{f}/R; R is the ideal gas constant, \Delta H\textsubscript{f} = 28 ± 3 kJ/mol, \Delta S\textsubscript{f} = 0.06 ± 0.01 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K\textsubscript{ow}:
5.88 (calculated-TSA, Burkhard 1984)
5.98 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
6.05 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.23 (Hawker & Connell 1988b)
5.90 (calculated-QSPR, Murray & Andren 1992)
Octanol/Air Partition Coefficient, log \( K_{OA} \):
- 8.93 (recommended, Sangster 1993)
- 6.0763 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Bioconcentration Factor, log BCF or log \( K_B \):

Sorption Partition Coefficient, log \( K_{OC} \):
- 5.68 (suspended particulate matter, Burkhard 1984)
- 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO\(_3\) radical and \( k_{O_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:
  \[ k_{OH}(calc) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
- \( k_1 = 0.005 \text{ d}^{-1} \) with \( t_{\frac{1}{2}} = 153 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.004 \text{ d}^{-1} \) with \( t_{\frac{1}{2}} = 164 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from \( t_{\frac{1}{2}} = 4–11 \text{ d} \) in freshwater systems, \( t_{\frac{1}{2}} = 0.1–10 \text{ d} \) in cloud water, \( t_{\frac{1}{2}} > 1000 \text{ d} \) in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration \( t_{\frac{1}{2}} = 153 \text{ d} \) for high-dose treatment, \( t_{\frac{1}{2}} = 164 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.77 3,3′,4,4′-Tetrachlorobiphenyl (PCB-77)

Common Name: 3,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-77, 3,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-13-3
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988
Melting Point (°C):
180 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2024
Molar Volume (cm³/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
27.10 (Ruelle et al. 1993)
Entropy of Fusion, ΔS_fus (J/mol K):
56.6 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.029 (calculated, assuming ΔS_fus = 56 J/mol K, Shiu & Mackay 1986)
0.0202 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.175 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
7.50 × 10⁻⁴ (generator column-GC/ECD, Weil et al. 1974)
5.69 × 10⁻⁴ (generator column-GC/ECD, measured 4–32°C, Dickhut et al. 1986)
5.84 × 10⁻⁴ (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
ln x = −6098/(T/K) – 3.586, temp range 4–32°C, ΔH_s = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = −2636/(T/K) – 1.558, ΔH_s = 50.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 3.59 × 10⁻¹⁰ exp(0.072·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
8.23 × 10⁻¹⁴, 1.01 × 10⁻¹³, 1.16 × 10⁻¹³ (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
0.0018 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
5.50 × 10⁻⁴; 0.0161 (generator column-GC; supercooled liquid S_L, Dunnivant & Elzerman 1988)
6.10 × 10⁻⁴ (generator column-GC/ECD, room temp., Hong & Qiao 1995)
2.02 × 10⁻³, 5.44 × 10⁻³ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
log S_L (mol/L) = −0.246 + 1339/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = −3.58245 − 6074.34/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.00270* (generator column-GC/ECD, measured range 5–35°C. Huang & Hong 2002).—See Comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00219, 0.00196 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.0014 (supercooled liquid P_L, GT-RT correlation, Burkhard 1984)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- **4.37** (calculated-P/C, Burkhard et al. 1985b)
- **1.72** (calculated-P/C, Shiu & Mackay 1986)
- **9.52** (gas stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
- **40.88** (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
- **10.39** (calculated-QSPR, Dunnivant et al. 1992)
- **log H (Pa m³/mol) = 12.86 – 3214/(T/K); temp range: 4–31°C** (gas stripping-GC, Bamford et al. 2000)
- **ln K_{AW} = 11.0657 – 4787.1/(T/K); temp range: 4–31°C** (gas stripping-GC, Bamford et al. 2000)
- **ln K_{AW} = –(39.8/kJ·mol⁻¹)/RT + (0.092/kJ·mol⁻¹·K⁻¹)/R; R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C** (gas stripping-GC, Bamford et al. 2000)
- **16.7** (exptl. data, Bamford et al. 2002)
- **ln K_{AW} = –\Delta H_{g}/RT + \Delta S_{g}/R; R is the ideal gas constant, \Delta H_{g} = 40 ± 6 kJ/mol, \Delta S_{g} = 0.09 ± 0.02 kJ/mol·K** (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:

- **6.04** (HPLC-RT correlation, Sugiuira et al. 1979)
- **6.52** (RP-TLC-retention, Bruggeman et al. 1982)
- **5.62** (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- **6.77** (HPLC-k' correlation, De Kock & Lord 1987)
- **6.11, 6.40, 6.37** (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- **6.21** (generator column-GC, Hawker & Connell 1988a)
- **6.630 ± 0.018** (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- **6.13** (generator column-GC, Larsen et al. 1992)
- **5.98** (HPLC-k' correlation, Noegrohati & Hammers 1992)
- **7.8733** (calculated-UNIFAC group contribution, Chen et al. 1993)
- **6.11** (recommended, Sangster 1993)
- **6.63** (recommended, Hansch et al. 1995)
- **6.48** (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- **9.08** (calculated, Paterson et al. 1991)
- **9.96** (20°C, generator column-GC, measured range 0 to 30°C, Harner & Bidleman 1996)
- log K_{oa} = –3.14 + 3828/(T/K); (temp range 0 to 30°C, Harner & Bidleman 1996)
- **10.92, 9.92; 10.03 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)**
Polychlorinated Biphenyls (PCBs)

9.70  (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.29; 9.19 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Species/Condition</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.46</td>
<td>killifish, Goto et al. 1978</td>
<td></td>
</tr>
<tr>
<td>3.90, 3.24, 3.63, 4.15</td>
<td>golden orfe, carp, brown trout, guppy, Sugiura et al. 1979</td>
<td></td>
</tr>
<tr>
<td>2.77, 2.63</td>
<td>(human fat in lipid, wet wt. basis, calculated-K&lt;sub&gt;OW&lt;/sub&gt;, Geyer et al. 1987)</td>
<td></td>
</tr>
<tr>
<td>5.36; 6.89</td>
<td>(22°C, zebrafish: log BCF&lt;sub&gt;W&lt;/sub&gt; wet wt basis; log BCF&lt;sub&gt;L&lt;/sub&gt; lipid wt basis, Fox et al. 1994)</td>
<td></td>
</tr>
<tr>
<td>4.59, 5.87, 4.745, 4.943</td>
<td>(quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K&lt;sub&gt;OW&lt;/sub&gt;, Lu et al. 1999)</td>
<td></td>
</tr>
<tr>
<td>2.56–4.26</td>
<td>(various marine species, mean dry wt. BCF, Hope et al. 1998)</td>
<td></td>
</tr>
<tr>
<td>4.19–5.23</td>
<td>(various marine species, mean lipid-normalized BCF, Hope et al. 1998)</td>
<td></td>
</tr>
<tr>
<td>3.56</td>
<td>(Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)</td>
<td></td>
</tr>
<tr>
<td>5.36, 6.90</td>
<td>(zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
<td></td>
</tr>
<tr>
<td>4.41, 6.37</td>
<td>(mussel Mytilus edulis: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
<td></td>
</tr>
<tr>
<td>2.62, 2.77</td>
<td>(human: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
<td></td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log K<sub>OC</sub>:

<table>
<thead>
<tr>
<th>Value</th>
<th>Condition</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.75</td>
<td>(suspended particulate matter, calculated-K&lt;sub&gt;OW&lt;/sub&gt;, Burkhard 1984)</td>
<td></td>
</tr>
<tr>
<td>4.41</td>
<td>(soil, calculated, Chou &amp; Griffin 1986)</td>
<td></td>
</tr>
<tr>
<td>5.02</td>
<td>(soil, calculated-QSPR Characteristic Root Index CRI, Saçan &amp; Balcioğlu 1996)</td>
<td></td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>½</sub>:

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant k, for gas-phase second order rate constants, k<sub>OH</sub> for reaction with OH radical, k<sub>NO<sub>3</sub></sub> with NO<sub>3</sub> radical and k<sub>O3</sub> with O<sub>3</sub> or as indicated, *data at other temperatures see reference:
  - k<sub>OH</sub>(calc) = (0.4 – 0.9) × 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>–1</sup> s<sup>–1</sup> for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - k<sub>OH</sub>(calc) = (0.36 – 1.7) × 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>–1</sup> s<sup>–1</sup> for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:
  - k<sub>1</sub> = 0.029, 0.0047 d<sup>–1</sup> (golden orfe, guppy, Sugiura et al. 1979)
  - k<sub>2</sub> = 0.0157 d<sup>–1</sup> (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
  - k<sub>1</sub> = 5160 d<sup>–1</sup>; k<sub>2</sub> = 0.0224 d<sup>–1</sup> (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
  - k<sub>1</sub> = 17 L d<sup>–1</sup> g<sup>–1</sup> dry wt.; k<sub>2</sub> = 0.073 d<sup>–1</sup> (Baltic Sea blue mussel, flow-through expt., Gustafsson et al. 1999)
  - k<sub>1</sub> = 0.0251 d<sup>–1</sup> with t<sub>½</sub> = 28 d (newly contaminated oysters, Gardinali et al. 2004)
  - k<sub>2</sub> = 0.0166 d<sup>–1</sup> with t<sub>½</sub> = 42 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995);
- t<sub>½</sub> = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
- Surface water: t<sub>½</sub> = 805 d in Lake Michigan (Neely 1983);
- photodegradation t<sub>½</sub> = 528 min when irradiated in a TiO<sub>2</sub> semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
- t<sub>½</sub> = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: $t_{1/2} = 87600\ h$ at $7^\circ C$ for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{1/2} = 87600\ h$ at $7^\circ C$ for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: $t_{1/2} = 44\ d$ in rainbow trout, and its muscle, $29\ d$ (Niimi & Oliver 1983);
theoretical half-life to reach 90% steady-state tissue concn $9.5\ d$ (Baltic Sea blue mussels, flow-through exp., Gustafsson et al. 1999)
Depuration $t_{1/2} = 28\ d$ for newly contaminated oysters, and $t_{1/2} = 42\ d$ for chronically contaminated oysters (Gardinali et al. 2004)

### TABLE 7.1.1.77.1
Reported aqueous solubilities, Henry’s law constants and octanol-air partition coefficients of 3,3′,4,4′-tetrachlorobiphenyl (PCB 77) at various temperatures and the reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>Henry’s law constant</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$S/g\cdot m^{-3}$</td>
<td>$t/°C$</td>
<td>$H/(Pa\ m^3/mol)$</td>
</tr>
<tr>
<td>4</td>
<td>$1.46 \times 10^{-4}$</td>
<td>5</td>
<td>4</td>
</tr>
<tr>
<td>20</td>
<td>$4.38 \times 10^{-4}$</td>
<td>15</td>
<td>11</td>
</tr>
<tr>
<td>25</td>
<td>$5.84 \times 10^{-4}$</td>
<td>25</td>
<td>18</td>
</tr>
<tr>
<td>32</td>
<td>$1.17 \times 10^{-3}$</td>
<td>35</td>
<td>25</td>
</tr>
</tbody>
</table>

$ln\ x = A - B/(T/K)$, $mp/°C = 180-181$

$\Delta H_{sol}/(kJ\ mol^{-1}) = 29.6$

enthalpy of solution:
$\Delta H_{sol}/(kJ\ mol^{-1}) = 50.7 \pm 4.8$

for 4–32°C

$ln\ K_{AW} = -\Delta H/RT + \Delta S/R$

<table>
<thead>
<tr>
<th></th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>10.88</td>
</tr>
<tr>
<td>20</td>
<td>10.36</td>
</tr>
<tr>
<td>25</td>
<td>9.75</td>
</tr>
<tr>
<td>32</td>
<td>9.47</td>
</tr>
</tbody>
</table>

$\Delta H_{OA}/(kJ\ mol^{-1}) = 73.30$

$\Delta H/(kJ\ mol^{-1}) = 39.8 \pm 6.0$

$\Delta S/(J\cdot mol^{-1}\cdot K^{-1}) = 92 \pm 20$

$log K_{OA} = A + B/T$

A $= -3.14$

B $= 3828$
FIGURE 7.1.1.77.1 Logarithm of mole fraction solubility, Henry's law constant and $K_{OA}$ versus reciprocal temperature for 3,3',4,4'-tetrachlorobiphenyl (PCB-77).
7.1.1.78 3,3′,4,5-Tetrachlorobiphenyl (PCB-78)

Chemical Name: 3,3′,4,5-tetrachlorobiphenyl
CAS Registry No: 70362-49-1
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988

Melting Point (°C): 94 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0943 (\( S_L \) supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00186 (\( P_L \) supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00116, 0.000167, 0.000223 (calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985b)
0.00319, 0.00206 (supercooled liquid \( P_L \), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
\[
\log \left( \frac{P_l}{P_a} \right) = -4598/T + 12.92 \quad (\text{GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994})
\]

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
5.76 (calculated-P/C, Burkhard 1984)
22.90 (calculated-QSPR-MCI \( \chi \), Sabljic & Güsten 1989)
21.77 (calculated-QSPR, Dunivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\[
\ln K_{\text{AW}} = -\Delta H_{\text{ fus}}/RT + \Delta S_{\text{ fus}}/R; \quad R \text{ is the ideal gas constant, } \Delta H_{\text{ fus}} = 36 \pm 5 \text{ kJ/mol, } \Delta S_{\text{ fus}} = 0.08 \pm 0.01 \text{ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004}
\]

Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
5.95 (calculated, Burkhard 1984)
6.35 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2278 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):

Bioconcentration Factor, log BCF or log \( K_{\text{bc}} \):

Sorption Partition Coefficient, log \( K_{\text{oc}} \):
5.75 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}$(calc) = (0.4–0.9) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987).

$k_{OH}$(calc) = (0.36–1.7) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 8.5–40 d at room temp. (Kwok et al. 1995).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1$: 8 (food lipid mg)/(g worm lipid-d);
- $k_2$: 0.09 d$^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 7$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.79 3,3′,4,5′-Tetrachlorobiphenyl (PCB-79)

Common Name: 3,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-79
Chemical Name: 3,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 41464-48-6
Molecular Formula: C_{12}H_6Cl_4
Molecular Weight: 291.988
Melting Point (°C): 83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0815 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0036 (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.07 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00224, 0.00184 (calculated-MW, GC-RÍ correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00341, 0.00206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = –4598/(T/K) + 12.95 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
7.39 (calculated-P/C, Burkhard 1984)
11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.94 (calculated-QSPR, Achman et al. 1993)
12.73 (calculated-QSAR, Dunnivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 36 ± 5 kJ/mol, ΔS_{f} = 0.08 ± 0.01 kJ/mol-K
(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Octanol/Water Partition Coefficient, log K_{ow}:
6.00 (calculated-TSA, Burkhard 1984)
6.3035 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
9.67 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{bi}:
Polychlorinated Biphenyls (PCBs)

Sorption Partition Coefficient, log $K_{OC}$:
5.80 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $\tau$:
- **Volatilization:**
- **Photolysis:**
- **Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  
  $k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  
  $k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5–40$ d at room temp. (Kwok et al. 1995)

- **Hydrolysis:**
- **Biodegradation:**
- **Biotransformation:**
- **Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

Half-Lives in the Environment:
- **Air:** calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
  
  tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

- **Surface water:**
- **Ground water:**
- **Sediment:**
- **Soil:**
- **Biota:**
7.1.1.80 3,3′,5,5′-Tetrachlorobiphenyl (PCB-80)

Common Name: 3,3′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-80, 3,3′,5,5′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,5,5′-tetrachlorobiphenyl
CAS Registry No: 33284-52-5
Molecular Formula: C₁₂H₆Cl₄
Molecular Weight: 291.988

Melting Point (°C):
164 (Van Roosmalen 1934; Hutzinger et al. 1974)

Boiling Point (°C):

Density (g/cm³):
- 268.2 (calculated-Le Bas method at normal boiling point)
- 211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.0421 (Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0712 (supercooled liquid Sₐ, calculated-TSA, Burkhard et al. 1985b)
- 0.000306, 0.000496, 0.000786, 0.000902 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.00124 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
- 0.0295 (supercooled liquid Sₐ, calculated-mp, Dunnivant & Elzerman 1988)
- 0.00292 (calculated-TSA, Abramowicz & Yalkowsky 1990)
- 2.92 × 10⁻³, 7.68 × 10⁻³ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- 4.96 × 10⁻³ (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.000859, 0.000139, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
- 0.00305 (supercooled liquid Pₐ, GC-RI correlation, Burkhard et al. 1985b)
- 0.00547, 0.00511 (supercooled liquid Pₐ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

log (Pₐ/Pa) = – 4598/(T/K) + 13.16 (supercooled liquid Pₐ, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 12.46 (calculated-P/C, Burkhard et al. 1985b)
- 63.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
- 38.0 (calculated-QSPR, Dunnivant et al. 1992)
- 20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln K_{AW} = –ΔH_{liq}/RT + ΔS_{liq}/R; R is the ideal gas constant, ΔH_{liq} = 36 ± 5 kJ/mol, ΔS_{liq} = 0.08 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
- 6.85 (HPLC-RT correlation, Sugiura et al. 1978; quoted, Hansch et al. 1995)
- 6.58 (RP-TLC-retention, Bruggeman et al. 1982)
Polychlorinated Biphenyls (PCBs)

6.77, 6.77, 6.45, 6.41 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.60 (recommended, Sangster 1993)
6.48, 6.85 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

9.26 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

5.85 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.4–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(calc) = (0.36–1.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 8.5–40$ d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:
7.1.1.81 3,4,4′,5-Tetrachlorobiphenyl (PCB-81)

Common Name: 3,4,4′,5-Tetrachlorobiphenyl
Synonym: PCB-81
Chemical Name: 3,4,4′,5-Tetrachlorobiphenyl
CAS Registry No: 70362-50-4
Molecular Formula: C12H6Cl4
Molecular Weight: 291.988
Melting Point (°C):
   137 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm3):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘₚ (kJ/mol):
Entropy of Fusion, ∆Sₘₚ (J/mol K):
Fugacity Ratio at 25°C, F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
   0.0929 (Sₜ, supercooled liquid, calculated-TSA, Burkhard et al. 1985)
   0.00292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
   0.0010 (room temp., generator column-GC/ECD, Hong & Qiao 1995)—see comment by van Noort 2004
   0.00313 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)
   0.00140, 0.00213, 0.00313, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   0.00165 (Pₜ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
   0.0204, 0.0018, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
   0.00290, 0.00182. (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
   log (P_l/Pa) = –4598/(T/K) + 12.88 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   5.20 (calculated-P/C, Burkhard et al. 1985a)
   15.0 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
   10.06 (calculated-QSPR, Dunnivant et al. 1992)
   5.97 (calculated-QSPR, Achman et al. 1993)
   12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
   25.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln Kₚₐₙ = –ΔH/RT + ΔS/R; R is the ideal gas constant, ΔHₘₚ = 33 ± 3 kJ/mol, ΔSₘₚ = 0.07 ± 0.01 kJ/mol·K
   (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₐₕₚ:
   5.96 (calculated-TSA, Burkhard 1984)
   6.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
   6.53; 6.16 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
   6.64, 6.24 (calculated-MCI χ, calculated-molecular properties MNDO-MI method, Yeh & Hong 2002)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:

\[
9.88 \quad \text{(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)}
\]

Bioconcentration Factor, log BCF or log $K_B$:

\[
5.10, 6.40 \quad \text{(fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)}
\]

Sorption Partition Coefficient, log $K_{OC}$:

\[
5.76 \quad \text{(suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)}
\]

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O3$ with O$_3$ or as indicated, *data at other temperatures see reference:

\[
k_{OH}(\text{calc}) = (0.4–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 25–60 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}
\]

\[
k_{OH}(\text{calc}) = (0.36–1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{for tetrachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 8.5–40 \text{ d at room temp. (Kwok et al. 1995)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

\[
k_1 = 0.0185 \text{ d}^{-1} \quad \text{with } t_\frac{1}{2} = 37 \text{ d (newly contaminated oysters, Gardinali et al. 2004)}
\]

\[
k_2 = 0.0186 \text{ d}^{-1} \quad \text{with } t_\frac{1}{2} = 37 \text{ d (chronically contaminated oysters, Gardinali et al. 2004)}
\]

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: clearance $t_\frac{1}{2} = 21$ d in guppy for tetrachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for tetrachlorobiphenyls: $t_\frac{1}{2} = 2–290$ d in trout, $t_\frac{1}{2} = 29–127$ d in trout muscle; $t_\frac{1}{2} = 51–81$ d in goldfish, $t_\frac{1}{2} = 7–200$ d in carp and $t_\frac{1}{2} = 4–53$ d in guppy (Niimi 1987)

Depuration $t_\frac{1}{2} = 37$ d for newly contaminated oysters, and $t_\frac{1}{2} = 37$ d for chronically contaminated oysters (Gardinali et al. 2004)
7.1.1.82 2,2',3,3',4-Pentachlorobiphenyl (PCB-82)

Common Name: 2,2',3,3',4-Pentachlorobiphenyl
Synonym: PCB-82
Chemical Name: 2,2',3,3',4-pentachlorobiphenyl
CAS Registry No: 52663-62-4
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C): 85 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0467 (S̄L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0291 (20°C, supercooled liquid, Murphy et al. 1987)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0028 (calculated-QSPR, Dunnivant et al. 1992)
0.00622 (calculated-group contribution method, Kühne et al. 1995)
0.0221 (calculated-mp and K_{OW}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0020 (P̄L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00218, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.06 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)
Henry’s Law Constant (Pa⋅m³/mol at 25°C or as indicated):
12.46 (calculated-P/C, Burkhard 1984)
11.86 (20°C, calculated-P/C, Murphy et al. 1987)
12.36 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.82 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
16.3 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = -\Delta H_{fus}/RT + \Delta S_{fus}/R; R is the ideal gas constant, \Delta H_{fus} = 42 ± 8 kJ/mol, \Delta S_{fus} = 0.11 ± 0.03 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
6.20 (calculated-TSA, Burkhard 1984)
6.30 (estimated, Girvin & Scott 1997)
6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.73 (calculated-CLOGP ver. 4, Ran et al. 2002)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
6.00 (suspended particulate matter, Burkhard 1984)
4.770 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{ad}$, calculated-MCI $\chi$, Sabljic et al. 1989)
5.80 (soil, calculated-$K_{ow}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}$(calc) = (0.2–0.4) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}$(calc) = (0.3–0.9) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_2 = 0.004$ d$^{-1}$ with $t_{\frac{1}{2}} = 174$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d$^{-1}$ with $t_{\frac{1}{2}} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{\frac{1}{2}} = 174$ d for high-dose treatment, $t_{\frac{1}{2}} = 196$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.83 2,2′,3,3′,5-Pentachlorobiphenyl (PCB-83)

Common Name: 2,2′,3,3′,5-Pentachlorobiphenyl
Synonym: PCB-83
Chemical Name: 2,2′,3,3′,5-pentachlorobiphenyl
CAS Registry No: 60145-20-2
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C): 65 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle et al. 1997)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.405 (mp at 65°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0045 (generator column-GC/ECD, Weil et al. 1974)
0.023 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.046 (supercooled liquid $S_1$, calculated-TSA, Burkhard et al. 1985b)
0.0282 (20°C, supercooled liquid $S_1$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0260 (calculated-TSA, Abramowitcz & Yalkowsky 1990)
0.0103, 0.0278 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00735, 0.00324, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985a)
0.00299 (supercooled liquid $P_l$, GC-R/I correlation, Burkhard et al. 1985b)
0.00274, 0.00303 (supercooled liquid $P_l$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00154 (20°C, supercooled liquid $P_l$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.0 - 4760/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00204 (supercooled liquid $P_l$: GC-R/I correlation, Fischer et al. 1992)
log ($P_l/P_a$) = -4522/(T/K) + 12.60 (supercooled liquid $P_l$, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
21.28 (calculated-P/C, Burkhard et al. 1985b)
16.62 (20°C, calculated-P/C, Murphy et al. 1987)
26.65 (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
21.46 (calculated-QSPR, Dunnivant et al. 1992)
23.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_g/RT + \Delta S_g/R$; R is the ideal gas constant, $\Delta H_g = 30 \pm 6$ kJ/mol, $\Delta S_g = 0.07 \pm 0.02$ kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.24 (calculated-TSA, Burkhard 1984)
- 6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.51 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
- 6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.44, 9.39 (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
- 9.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.04 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 4.748 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis: Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$ k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 60-120 \text{ d, due to gas-phase loss process at room temp.} \text{ (Atkinson 1987) }$$

$$ k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 16-48 \text{ d at room temp.} \text{ (Kwok et al. 1995) }$$

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004) }$
- $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 217 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004) }$

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1996).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 172 \text{ d for high-dose treatment, } t_{1/2} = 217 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004) }$
7.1.1.84 2,2',3,3',6-Pentachlorobiphenyl (PCB-84)

Common Name: 2,2',3,3',6-Pentachlorobiphenyl
Synonym: PCB-84, 2,2',3,3',6-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',6-pentachlorobiphenyl
CAS Registry No: 52663-60-2
Molecular Formula: C_{12}H_5Cl_5
Molecular Weight: 326.433

Melting Point (°C): 91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.047 (20°C, supercooled liquid, Murphy et al. 1987)
  0.0542 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
  0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  6.48 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00735, 0.00693, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00372, 0.00441 supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  2.64 × 10⁻³ (20°C, supercooled liquid, Murphy et al. 1987)
  log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
  0.00302, 0.0055 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
  log (P_L/Pa) = –4399/(T/K) + 12.32 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  51.68 (calculated-P/C, Burkhard 1984)
  17.63 (20°C, calculated-P/C, Murphy et al. 1987)
  24.82 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
  5.97 (calculated-QSPR, Achman et al. 1993)
  25.45 (calculated-QSPR, Dunnivant et al. 1992)
  51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 18 ± 6 kJ/mol, ΔS_{f} = 0.03 ± 0.01 kJ/mol·K
  (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
  6.04 (RP-HPLC-k’ correlation, Rapaport & Eisenreich 1984)
  5.60 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
  6.24 (generator column-GC, Larsen et al. 1992)
  5.96 (recommended, Sangster 1993)
  6.04 (recommended, Hansch et al. 1995)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.80 (quoted, Kömp & McLachlan 1997b)
- 10.28, 9.28 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 8.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Biota Sediment Accumulation Factor, BSAF:
- 80 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.09 (suspended particulate matter, Bukhard 1984)
- 4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volutilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH}$(calc) = (0.2–0.4) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}$(aq.) = 4.7 × 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_\frac{1}{2} \sim 4–11$ d in freshwater systems, $t_\frac{1}{2} = 0.1–10$ d in cloud water, $t_\frac{1}{2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1 = 0.005 \text{ d}^{-1}$ with $t_\frac{1}{2} = 135$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.005 \text{ d}^{-1}$ with $t_\frac{1}{2} = 141$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_\frac{1}{2} \sim 4–11$ d in freshwater systems, $t_\frac{1}{2} = 0.1–10$ d in cloud water, $t_\frac{1}{2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration $t_\frac{1}{2} = 135$ d for high-dose treatment, $t_\frac{1}{2} = 141$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.85 2,2′,3,4,4′-Pentachlorobiphenyl (PCB-85)

Common Name: 2,2′,3,4,4′-Pentachlorobiphenyl
Synonym: PCB-85, 2,2′,3,4,4′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′-pentachlorobiphenyl
CAS Registry No: 65510-45-4
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
  87  (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  289.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  0.0428  (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.0219  (20°C, supercooled liquid, Murphy et al. 1987)
  0.00782  (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  0.0130  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.00233  (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  0.00735, 0.00253, 0.000532  (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
  0.00472, 0.00218  (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  1.12 × 10⁻³  (20°C, supercooled liquid, Murphy et al. 1987)
  log (P_L/Pa) = –4522/(T/K) + 12.54  (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
  0.00248  (P_L, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  17.83  (calculated-P/C, Burkhard 1984)
  16.72  (20°C, calculated-P/C, Murphy et al. 1987)
  24.82  (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  6.69  (wetted-wall column-GC/ECD, Brunner et al. 1990)
  19.49  (calculated-QSPR, Dunnivant et al. 1992)
  26.4  (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  47.2  (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_fus/RT + ΔS_fus/R; R is the ideal gas constant, ΔH_fus = 26 ± 7 kJ/mol, ΔS_fus = 0.05 ± 0.02 kJ/mol·K  (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
  6.61  (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
  6.18  (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
  6.63  (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
  6.18  (recommended, Sangster 1993)
  6.61  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

9.29 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.07 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_W$, calculated-MCI $\chi$, Sabljic et al. 1989)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.70 (soil-organic carbon, Girvin & Scott 1997)
- 5.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.70 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH}$(calc) = (0.2–0.4) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}$(calc) = (0.3–0.9) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.86 2,2',3,4,5-Pentachlorobiphenyl (PCB-86)

Common Name: 2,2',3,4,5-Pentachlorobiphenyl
Synonym: PCB-86, 2,2',3,4,5-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,5-pentachlorobiphenyl
CAS Registry No: 55312-69-1
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433

Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
0.0098 (generator column-GC/ECD, Weil et al. 1974)
0.0349 (generator column-HPLC/UV, Huang 1983)
0.034 (generator column-HPLC, Billington et al. 1988)
0.00334, 0.00554, 0.00297, 0.00651 (RP-HPLC-k correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00933 (quoted, Neely 1981)
0.051 (P_{L} calculated from P_{S} using fugacity ratio F, Neely 1981)
0.00643 (supercooled liquid P_{L}, Neely 1981)
0.000077 (calculated, Neely 1983; quoted, Erickson 1986)
0.00133, 0.00245, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI \chi, Burkhard et al. 1985a)
0.0128 (supercooled liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)
0.00288 (supercooled liquid P_{L}, GC-RI correlations, Fischer et al. 1992)
log (P_{L}/Pa) = – 4522/(T/K) + 12.61 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
84.1 (calculated-P/C, Burkhard et al. 1985b)
17.23 (calculated-MCI \chi, Sabljic & Güsten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\ln K_{AW} = -\Delta H_{fust}/RT + \Delta S_{fust}/R; \ R \ is \ the \ ideal \ gas \ constant, \ \Delta H_{fust} = 29 \pm 8 \ \text{kJ/mol}, \ \Delta S_{fust} = 0.06 \pm 0.01 \ \text{kJ/mol·K} \ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (Neely 1983; quoted, Erickson 1986)
7.49 (calculated-fragment const., Yalkowsky et al. 1983)
6.22 (calculated-TSA, Burkhard 1984)
Polychlorinated Biphenyls (PCBs)

6.38 (calculated-π const., Woodburn et al. 1984)
6.20 (selected, Shiu & Mackay 1986)
6.44, 6.38, 6.43, 6.29 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.26 (calculated-MCI χ, Patil 1991)
6.39 (recommended, Sangster 1993)
6.325 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.97 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/air Partition Coefficient, log $K_{OA}$:
9.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.43 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)

Sorption Partition Coefficient, log $K_{OC}$:
6.02 (suspended particulate matter, calculated-$K_{OC}$, Burkhard 1984)
4.770 (marine humic substances, calculated-MCI χ, reported as log $K_h$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}^{calc} = (0.2 – 0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau^{calc}$ = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}^{calc} = (0.3 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau^{calc}$ = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.005 yr$^{-1}$ in the water column and k = 0.05 yr$^{-1}$ in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:
Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 108 d in Lake Michigan (Neely 1983).

Groundwater:
Sediment:
Soil:
Biota:
7.1.1.87 2,2',3,4,5'-Pentachlorobiphenyl (PCB-87)

Common Name: 2,2',3,4,5'-Pentachlorobiphenyl
Synonym: PCB-87, 2,2',3,4,5'-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,5'-pentachlorobiphenyl
CAS Registry No: 38380-02-8
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
- 111.5–113 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2803
Molar Volume (cm³/mol):
- 289.1 (calculated-Le Bas method at normal boiling point)
- 224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_\text{fus} (kJ/mol):
Entropy of Fusion, ΔS_\text{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_\text{fus} = 56 J/mol K), F:
- 0.132 (Mackay et al. 1980)
- 0.138 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.022 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.0045 (generator column-GC/ECD, Weil et al. 1974)
- 0.0294 (20°C, supercooled liquid S₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.0082, 0.00783, 0.00543, 0.0070 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.00226 (supercooled liquid P₁, GC-RT correlation, Bidleman 1984)
- 0.000392 (GC-RI correlation, Burkhard et al. 1985a)
- 0.00141, 0.00262 (supercooled liquid P₁, GC-RI correlation, Burkhard et al. 1985b)
- 0.00261, 0.00248 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.00116 (20°C, supercooled liquid P₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.10 – 4800/(T/K) (GC-RT correlation, Tateya et al. 1988)
- 0.0017, 0.00275 (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P₁/Pa) = – 4562/(T/K) + 12.66 (supercooled liquid P₁, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
- 33.44 (calculated, Murphy et al. 1983)
- 19.86 (calculated-P/C, Burkhard et al. 1985b)
- 24.81 (calculated-P/C, Shiu & Mackay 1986)
- 12.87 (20°C, calculated-P/C, Murphy et al. 1987)
- 18.24 (calculated-QSAR-MCl χ, Sabljic & Güsten 1989)
- 7.50 (wetted-wall column-GC, Brunner et al. 1990)
- 18.61 (calculated-QSPR, Dunnivant et al. 1992)
- 5.966 (calculated-QSPR, Achman et al. 1993)
Polychlorinated Biphenyls (PCBs)

37.71 ± 0.69 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln $K_{AW} = 8.9006 - \frac{3909.07}{(T/K)}$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(32.5/kJ\cdot mol^{-1})/RT] + (0.074/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314$ J·K$^{-1}$·mol$^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.5 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_f/RT + \Delta S_f/R$; $R$ is the ideal gas constant, $\Delta H_f = 33 ± 4$ kJ/mol, $\Delta S_f = 0.07 ± 0.01$ kJ/mol·K—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{OW}$:
6.85 (RP-TLC-$k'$ correlation, Bruggeman et al. 1982)
6.30 (HPLC-RT correlation, Shaw & Connell 1982)
5.45, 6.37 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.14, 6.23, 6.24, 6.27 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.36 (HPLC-$k'$ correlation, Noegrohati & Hammers 1992)
6.23 (recommended, Sangster 1993)
6.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
9.96 (10°C, estimated, Thomas et al. 1998)
9.25 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
4.43 (oyster, Vreeland 1974)
5.38; 6.91 (22°C, zebrafish: log $BCF_W$ wet wt basis; log $BCF_L$ lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:
4.54 (Koch 1983)
6.07 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
4.88 (calculated, Bahnick & Doucette 1988)
4.761, 4.748 (marine humic substances of 5 mg/L DOC, selected, calculated-MCI $\chi$, reported as log $K_p$, Sabljic et al. 1989)
4.76, 4.87, 4.85, 3.75 (marine humic substance in concentrations of 5,10, 20, 40 mg/L DOC, reported as log $K_p$, Lara & Ernst 1989)
6.18 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.08 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.73 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted and selected, Baker et al. 2000)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.62 (soil, calculated-MCI, Sabljic et al. 1995)
5.02 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
6.00 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
5.80; 4.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Sorption Partition Coefficient, log $K_{OM}$:
4.50, 4.85 (selected, calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k_r$ for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated. *data at other temperatures see reference:

$k_{OH}(calc) = (0.2 – 0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3 – 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_2 = 0.0045$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
- $k_1 = 0.049$ h$^{-1}$; $k_2 = 0.013$ h$^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)
- $k_1 = 3360$ d$^{-1}$; $k_2 = 0.0140$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 154$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 195$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants $k_d$ for labile PCBs sorbed to utility substation soils are: $k = 0.027$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.57$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and $k = 0.27$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants $k_d$ for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00152$ d$^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00223$ d$^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and $k = 0.0039$ d$^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{1/2} = 155$ d in rainbow trout and $t_{1/2} = 62$ d its muscle (Niimi & Oliver 1983).

depuration $t_{1/2} = 154$ d for high-dose treatment, $t_{1/2} = 195$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
### 2,2′,3,4,6-Pentachlorobiphenyl (PCB-88)

**Common Name:** 2,2′,3,4,6-Pentachlorobiphenyl  
**Synonym:** PCB-88  
**Chemical Name:** 2,2′,3,4,6-pentachlorobiphenyl  
**CAS Registry No:** 55215-17-3  
**Molecular Formula:** C₁₂H₅Cl₅  
**Molecular Weight:** 326.433  
**Melting Point (°C):** 100  
(Mackay et al. 1980; Burkhard et al. 1985a; Oppenhuizen et al. 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):** 1.2803  
**Molar Volume (cm³/mol):**  
- 289.1 (calculated-Le Bas method at normal boiling point)  
- 224.5 (Ruelle & Kesselring 1997)  
**Enthalpy of Fusion, Δₕₜₕ (kJ/mol):**  
**Entropy of Fusion, Δₛₜₕ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming Δₛₜₕ = 56 J/mol K), F:** 0.182  
(Mackay et al. 1980)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
- 0.012 (generator column-GC/ECD, Weil et al. 1974)  
- 0.0129 (calculated-TSA, Mackay et al. 1980)  
- 0.0385 (supercooled liquid Sₗ, calculated-TSA, Burkhard et al. 1985b)  
- 0.00242 (calculated-fragment solubility constants, Wakita et al. 1986)  
- 0.009 (calculated-MCI χ, Nirmalakhandan & Speece 1989)  
- 0.0206 (calculated-TSA, Abramowitz & Yalkowsky 1990)  
- 0.011 (calculated-MCI χ, Patil 1991)  
- 0.00801 (calculated-group contribution, Kühne et al. 1995)  
- 0.0124, 0.00472 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
- 0.0265 (calculated-mp and K_OW, Ran et al. 2002)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
- 0.00309 (GC-RI correlation, Burkhard et al. 1985a)  
- 0.0161 (supercooled liquid Pₗ, GC-RI correlation, Burkhard et al. 1985b)  
- 0.00646 (supercooled liquid Pₗ, GC-RI correlation, Fischer et al. 1992)  
\[
\log (Pₗ/Pₐ) = -4399/(T/K) + 12.53 \quad \text{(supercooled liquid Pₗ, GC-RT correlation, Falconer & Bidleman 1994)}
\]  
**Henry’s Law Constant (Pa m³/mol at 25°C):**  
- 136.8 (calculated-P/C, Burkhard et al. 1985b)  
- 34.65 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)  
- 38.97 (calculated-QSPR, Dunnivant et al. 1992)  
- 51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\[
\ln Kₐₖₐₜ = -\Delta Hᵣᵣ/RT + \Delta Sᵣᵣ/R; \quad \text{R is the ideal gas constant, } \Delta Hᵣᵣ = 18 \pm 6 \text{ kJ/mol, } \Delta Sᵣᵣ = 0.03 \pm 0.01 \text{ kJ/mol-K (Bamford et al. 2002)–see Comment by Goss et al. 2004} 
\]  
**Octanol/Water Partition Coefficient, log K_OW:**  
- 7.51 (calculated-fragment const., Yalkowsky et al. 1983)
Octanol/Air Partition Coefficient, log $K_{OA}$:
- 9.39 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.11 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 4.611 (marine humic substances, calculated-MCI $\chi$, reported as association coefficient log $K_h$ at 5 mg/L of DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:
  $k_{OH}$(calc) = (0.2–0.4) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
  $k_{OH}$(calc) = (0.3–0.9) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
  tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
7.1.1.89 2,2',3,4,6'-Pentachlorobiphenyl (PCB-89)

Common Name: 2,2',3,4,6'-Pentachlorobiphenyl
Synonym: PCB-89, 2,2',3,4,6'-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,6'-pentachlorobiphenyl
CAS Registry No: 73575-57-2
Molecular Formula: C\textsubscript{12}H\textsubscript{5}Cl\textsubscript{5}
Molecular Weight: 326.433
Melting Point (°C): 99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}): 289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH\textsubscript{ fus} (kJ/mol):
Entropy of Fusion, ΔS\textsubscript{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS\textsubscript{ fus} = 56 J/mol K), F:

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
0.0382 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0542 (RP-HPLC-k correlation, Brodsky & Ballachmiter 1988)
0.0206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.82 \times 10\textsuperscript{-3} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00522 (GC-RI correlation, Burkhard et al. 1985b)

Henry’s Law Constant (Pa-m\textsuperscript{3}/mol at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard 1984)
29.49 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.18 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
30.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
\ln K_{AW} = -\Delta H_{g}/RT + \Delta S_{g}/R; R is the ideal gas constant, \Delta H_{g} = 21 \pm 6 \text{ kJ/mol}, \Delta S_{g} = 0.04 \pm 0.02 \text{ kJ/mol-K}
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K\textsubscript{ow}:
6.31 (calculated-TSA, Burkhard 1984)
6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.60 (RP-HPLC-k' correlation, Brodsky & Ballachmiter 1988)
6.40 (calculated-TSA, Murray & Andren 1992)
5.60 (recommended, Sangster 1993)
5.8981 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K\textsubscript{oa}:
9.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K\textsubscript{bi}:

© 2006 by Taylor & Francis Group, LLC
Sorption Partition Coefficient, log $K_{OC}$:

- 6.11 (suspended particulate matter, Burkhard 1984)
- 4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

### Volatilization:

### Photolysis:

### Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH(calc)} = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH(calc)} = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48 \text{ d}$ at room temp. (Kwok et al. 1995)

### Hydrolysis:

### Biodegradation:

### Biotransformation:

### Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

### Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.90  2,2′,3,4′,5-Pentachlorobiphenyl (PCB-90)

Common Name: 2,2′,3,4′,5-Pentachlorobiphenyl  
Synonym: PCB-90, 2,2′,3,4′,5-pentachloro-1,1′-biphenyl  
Chemical Name: 2,2′,3,4′,5-pentachlorobiphenyl  
CAS Registry No: 68194-07-0  
Molecular Formula: C₁₂H₅Cl₅  
Molecular Weight: 326.433  
Melting Point (°C): 67 (estimated, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ΔHₕₚ (kJ/mol):  
Entropy of Fusion, ΔSₕₚ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₕₚ = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
0.0375 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.01344 (20°C, supercooled liquid Sₗ, Murphy et al. 1987)  
0.00494 (RP-HPLC-k′ correlation, Brodsky & Ballischmier 1988)  
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
0.00714 (calculated-group contribution method, Kühne et al. 1995)  
0.00107, 0.00198 (generator column-GC/ECD, estimated, Hong & Qiao 1995)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
7.52 × 10⁻³ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00375 (GC-RI correlation, Burkhard et al. 1985b)  
log (P/mmHg) = 11.0 - 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)  
0.00347 (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)  
log (P₁/Pa) = - 4522/(T/K) + 12.69, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
30.19 (calculated-P/C, Burkhard 1984)  
39.11 (calculated-QSAR-MCI χ, Sablje & Güsten 1989)  
29.83 (calculated-QSPR, Dunnivant et al. 1992)  
44.8 (from 11°C exp. data and compensation point, Bamford et al. 2002)  
ln Kₜₕₕ = - ΔHₕₖ/RT + ΔSₕₖ/R; R is the ideal gas constant, ΔHₕₖ = 29 ± 8 kJ/mol, ΔSₕₖ = 0.06 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log Kₜₕₕ:  
6.32 (calculated-TSA, Burkhard 1984)  
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballischmier 1988a)  
6.32 (recommended, Sangster 1993)  
Octanol/Air Partition Coefficient, log Kₜₕₕ:  
8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log $\text{BCF} \text{ or log } K_b$: 

Sorption Partition Coefficient, log $K_{OC}$:
- 6.12 (suspended particulate matter, Burkhard 1984)
- 4.66, 4.68, 4.75, 3.75 (marine humic substance in concentrations of 5, 10, 20, 40 mg/L DOC, reported as log $K_h$, Lara & Ernst 1989)
- 4.659, 4.726 (marine humic substance, observed, calculated-MCI, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 60–120 \text{ d, due to gas-phase loss process at room temp.} \text{ (Atkinson 1987)}$$

$$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 16–48 \text{ d at room temp.} \text{ (Kwok et al. 1995)}$$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.91 2,2′,3,4′,6-Pentachlorobiphenyl (PCB-91)

Common Name: 2,2′,3,4′,6-Pentachlorobiphenyl  
Synonym: PCB-91, 2,2′,3,4′,6-pentachloro-1,1′-biphenyl  
Chemical Name: 2,2′,3,4′,6-pentachlorobiphenyl  
CAS Registry No: 58194-05-8  
Molecular Formula: C_{12}H_{5}Cl_{5}  
Molecular Weight: 326.433

Melting Point (°C):  
93 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.0336 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0395 (20°C, supercooled liquid, Murphy et al. 1987)
0.0221 (RP-HPLC-k correlation, Brodsky & Ballischmier 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

7.52 \times 10^{-3} (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00803 (GC-RI correlation, Burkhard et al. 1985b)
0.00487, 0.00667 (supercooled liquid P_l, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.32 \times 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0038, 0.00589 (supercooled liquid P_l, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_l/Pa) = –4399/(T/K) + 12.44 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

73.16 (calculated-P/C, Burkhard 1984)
27.46 (20°C, calculated-P/C, Murphy et al. 1987)
35.78 (calculated-QSAR-MCI $\chi$, Sablje & Güsten 1989)
12.16 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.05 (calculated-QSPR, Dunnivant et al. 1992)
9.03 (calculated-QSPR, Achman et al. 1993)
42.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
54.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

ln K_{AW} = -\Delta H_{fus}/RT + \Delta S_{fus}/R; R is the ideal gas constant, $\Delta H_{fus} = 10 \pm 5$ kJ/mol, $\Delta S_{fus} = 0.00 \pm 0.02$ kJ/mol-K

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

6.31 (RP-HPLC-k correlation, Rapaport & Eisenreich 1984)
6.31 (calculated-TSA, Burkhard 1984)

© 2006 by Taylor & Francis Group, LLC
Octanol/Air Partition Coefficient, $\log K_{OA}$:
9.07 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:
6.11 (suspended particulate matter, Burkhard 1984)
4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, $*$data at other temperatures see reference:

$\log k_{OH} (calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau (calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$\log k_{NO_3} (calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau (calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 10$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.08$ d$^{-1}$ (earthworm, Wågman et al. 2001)

$k_1 = 0.08$ d$^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d$^{-1}$ with $t_{1/2} = 217$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:

Biota: elimination $t_{1/2} = 8$ d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 166$ d for high-dose treatment, $t_{1/2} = 217$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.92 2,2',3,5,5'-Pentachlorobiphenyl (PCB-92)

Common Name: 2,2',3,5,5'-Pentachlorobiphenyl
Synonym: PCB-92, 2,2',3,5,5'-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,5,5'-pentachlorobiphenyl
CAS Registry No: 52663-61-3
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C): 53 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0379 (S_<L> supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00494 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.92 × 10⁻³ (P_<L> supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00422, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00394, 0.00458 (supercooled liquid P_<L>, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
log (P/Pa) = – 4522/(T/K) + 12.76 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
33.64 (calculated-P/C, Burkhard 1984)
32.63 (calculated-QSAR-MCI χ, Sabllic & Güsten 1989)
26.35 (calculated-QSPR, Dunning et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
28.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
48.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_ÅW = –ΔH/RT + ΔS/R; R is the ideal gas constant, ΔH = 24 ± 6 kJ/mol, ΔS = 0.05 ± 0.02 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
6.05, 6.97 (RP-HPLC-k' correlation:uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.32 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
6.11 (generator column-GC, Larsen et al. 1992)
6.32 (recommended, Sangster 1993)
6.97 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

6.11 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI \( \chi \), Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 0.005$ d$^{-1}$ with $t_\frac{1}{2} = 135$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d$^{-1}$ with $t_\frac{1}{2} = 141$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_\frac{1}{2} = 135$ d for high-dose treatment, $t_\frac{1}{2} = 141$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.93 2,2',3,5,6-Pentachlorobiphenyl (PCB-93)

- **Common Name:** 2,2',3,5,6-Pentachlorobiphenyl
- **Synonym:** PCB-93, 2,2',3,5,6-pentachloro-1,1'-biphenyl
- **Chemical Name:** 2,2',3,5,6-pentachlorobiphenyl
- **CAS Registry No:** 73575-56-1
- **Molecular Formula:** C\textsubscript{12}H\textsubscript{5}Cl\textsubscript{5}
- **Molecular Weight:** 326.433
- **Melting Point (°C):** 91 (estimated, Abramowitz & Yalkowsky 1990)
- **Boiling Point (°C):**
- **Density (g/cm\textsuperscript{3}):**
- **Molar Volume (cm\textsuperscript{3}/mol):** 289.1 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):**
- **Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K):**
- **Fugacity Ratio at 25°C (assuming ΔS\textsubscript{fus} = 56 J/mol K), F:**

- **Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):**
  - 0.0411 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  - 0.0149, 0.0164, 0.00986, 0.0119 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  - 0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

- **Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
  - 0.0151 (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  - 0.00735, 0.0160, 0.00419 (calculated-MW, GC-R-I correlation, calculated-MCI χ, Burkhard et al. 1985b)
  - 0.00708 (supercooled liquid P\textsubscript{L}, GC-R-I correlation, Fischer et al. 1992)
  - log (P\textsubscript{L}/Pa) = −4399/(T/K) + 12.57 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

- **Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C or as indicated):**
  - 120.6 (calculated-P/C, Burkhard 1984)
  - 34.49 (calculated-QSPR, Dunnivant et al. 1992)
  - 51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[
\ln K_{AW} = -\frac{\Delta H\textsubscript{fus}}{RT} + \frac{\Delta S\textsubscript{fus}}{R}; \text{ R is the ideal gas constant, } \Delta H\textsubscript{fus} = 18 \pm 6 \text{ kJ/mol, } \Delta S\textsubscript{fus} = 0.03 \pm 0.01 \text{ kJ/mol·K} \text{ (Bamford et al. 2002)—see Comment by Goss et al. 2004}
\]

- **Octanol/Water Partition Coefficient, log K\textsubscript{OW}:**
  - 6.29 (calculated-TSA, Burkhard 1984)
  - 5.99, 6.06, 6.07, 6.12 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  - 6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  - 6.06 (recommended, Sangster 1993)
  - 6.1176 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

- **Octanol/Air Partition Coefficient, log K\textsubscript{OA}:**
  - 8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.09 (suspended particulate matter, Burkhard 1984)
- 4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_w$, calculated-MCI $\chi_1^3$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.94 2,2′,3,5,6′-Pentachlorobiphenyl (PCB-94)

Common Name: 2,2′,3,5,6′-Pentachlorobiphenyl
Synonym: PCB-94
Chemical Name: 2,2′,3,5,6′-pentachlorobiphenyl
CAS Registry No: 73575-55-0
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433

Melting Point (°C):
79  (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1  (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0336  (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0259  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
7.24 × 10⁻³  (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00774, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
70.62  (calculated-P/C, Burkhard 1984)
43.98  (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69  (calculated-QSPR, Dunnivant et al. 1992)
51.2  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln Kₐₜₘ = −ΔH/RT + ΔS/R; R is the ideal gas constant, ΔHₗ = 18 ± 6 kJ/mol, ΔSₗ = 0.03 ± 0.01 kJ/mol K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log Kₐₜₙ:
6.36  (calculated-TSA, Burkhard 1984)
6.0371 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log Kₐₙₐ:
8.64  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log Kₘ:
Sorption Partition Coefficient, log Kₐₖₘ:
6.16  (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

- **Volutilization:**
- **Photolysis:**
- **Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:
  \[ k_{\text{OH}}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 60–120 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)} \]
  \[ k_{\text{OH}}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 16–48 \text{ d at room temp. (Kwok et al. 1995)} \]

- **Hydrolysis:**
- **Biodegradation:**
- **Biotransformation:**
- **Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

Half-Lives in the Environment:

- **Air:** calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

- **Surface water:**
- **Ground water:**
- **Sediment:**
- **Soil:**
- **Biota:**
7.1.1.95  2,2',3,5',6-Pentachlorobiphenyl (PCB-95)

Common Name: 2,2',3,5',6-Pentachlorobiphenyl
Synonym: PCB-95, 2,2',3,5',6-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',3,5',6-pentachlorobiphenyl
CAS Registry No: 38379-99-6
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C): 98.5–100 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔHₕus (kJ/mol):
Entropy of Fusion, ΔSₕus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕus = 56 J/mol K), F: 0.184 (mp at 100°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0336  (supercooled liquid S₁, calculated-TSA, Burkhard 1985b)
0.0541  (20°C, supercooled liquid S₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0291, 0.0216, 0.0192, 0.0156; 0.021 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0259  (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011   (calculated-MCI χ, Patil 1991)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00735, 0.00905, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00849  (supercooled liquid P₁, GC-RI correlation, Burkhard et al. 1985b)
0.00537, 0.00744 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00335  (20°C, supercooled liquid P₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00427, 0.00741 (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P₁/Pa) = – 4399/(T/K) + 12.48 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.00295  (20°C, supercooled liquid P₁, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
0.00211  (P₁, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry’s Law Constant (Pa m³/mol at 25°C):
82.78  (calculated-P/C, Burkhard 1985b)
20.06  (20°C, calculated-P/C, Murphy et al. 1987)
29.38  (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
30.39  (calculated-QSPR, Dunnivant et al. 1992)
30.8   (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.5   (from 11°C expit. data and compensation point, Bamford et al. 2002)
\ln K_{AW} = -\Delta H_W/RT + \Delta S_W/R; R is the ideal gas constant, \Delta H_W = 21 ± 5 kJ/mol, \Delta S_W = 0.04 ± 0.02 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:
5.18 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
5.67, 5.98, 5.86, 6.05 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.08 (generator column-GC, Larsen et al. 1992)
5.92 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:
9.06 (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
10.51, 9.06, 9.51, 9.06, 8.55 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
$\log K_{OA} = -4.30 + 3904/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
10.07, 9.06; 9.07 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
9.04 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
6.16 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
5.3–6.8, 6.1; 7.40 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
6.30 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.60, 4.66, 4.61, 3.70 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_a$, Lara & Ernst 1989)
4.603, 4.589 (marine humic substances, observed; calculated-MCI $\chi$, reported as association coefficient log $K_a$ at 5 mg/L DOC, Sabljic et al. 1989)
5.68, 5.70, 5.64 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.55 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_½:
Volatile:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

$k_1 = 0.00030$ h⁻¹; $k_2 = 0.184$ h⁻¹ (blood plasma of ring doves, Drouillard & Norstrom 2000)
$k_2 = 0.004$ d⁻¹ with $t_½ = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003$ d⁻¹ with $t_½ = 225$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 8.29$ min when irradiated in a TiO$_2$ semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 164$ d for high-dose treatment, $t_{1/2} = 225$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004).
7.1.1.96 2,2′,3,6,6′-Pentachlorobiphenyl (PCB-96)

Common Name: 2,2′,3,6,6′-Pentachlorobiphenyl
Synonym: PCB-96
Chemical Name: 2,2′,3,6,6′-pentachlorobiphenyl
CAS Registry No: 73575-54-9
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433

Melting Point (°C): 
53 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C): 

Density (g/cm³): 

Molar Volume (cm³/mol): 
289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol): 

Entropy of Fusion, ∆S_{fus} (J/mol K): 

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C): 
0.0368 (S₇ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C): 
0.0157 (P₇ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00166, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C): 
139.8 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
41.56 (calculated-QSPR, Dunnivant et al. 1992)
62.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\ln K_{AW} = - \Delta H_{f}/RT + \Delta S_{f}/R; R \text{ is the ideal gas constant, } \Delta H_{f} = 15 \pm 3 \text{ kJ/mol, } \Delta S_{f} = 0.02 \pm 0.01 \text{ kJ/mol·K} (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
6.33 (calculated-TSA, Burkhard 1984)
5.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hanch et al. 1995)
5.5365 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{oa} or as indicated and reported temperature dependence equations:
10.28, 9.72, 9.22, 8.77, 8.30 (~10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log K_{oa} = -4.60 + 3913/(T/K), temp range –10 to 30°C (Harner & Bidleman 1996)
9.87, 8.79; 8.76 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
8.82 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{bi}:

Sorption Partition Coefficient, log K_{oc}:
6.13 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constant and Half-Lives:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} for pentachlorobiphenyls, and the tropospheric lifetime \( \tau \) (calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} for pentachlorobiphenyls, and the tropospheric lifetime \( \tau \) (calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.97 2,2′,3,4′,5′-Pentachlorobiphenyl (PCB-97)

Common Name: 2,2′,3,4′,5′-Pentachloro
Synonym: PCB-97
Chemical Name: 2,2′,3,4,5-pentachlorobiphenyl
CAS Registry No: 41464-51-1
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
82 (Burkhard et al. 1984b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
53.77 (quoted, Shiu & Mackay 1986)
Fugacity Ratio at 25°C, F:
0.279 (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
0.0431 (\( S_L \) supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0284 (20°C, supercooled liquid, Murphy et al. 1987)
0.00622, 0.00651, 0.00383, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0099 (literature average, Paya-Perez et al. 1991)
0.00847 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.73 \times 10^{-3} (\( P_L \) supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.01 \times 10^{-3}, 8.05 \times 10^{-4}, 8.04 \times 10^{-3} (calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985b)
0.00251, 0.00265 (supercooled liquid \( P_L \), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.31 \times 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
\log (P/mmHg) = 11.10 – 4790/(T/K) (GC-RT correlation, Tateya et al. 1988)
1.85 \times 10^{-3}, 2.88 \times 10^{-3} (supercooled liquid \( P_L \), GC-RI correlation, different stationary phases, Fischer et al. 1992)
\log (P_L/Pa) = -4522/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0026 (\( P_L \), calculated-MCI \( \chi \) and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
20.67 (calculated-P/C, Burkhard 1984)
15.1 (20°C, calculated-P/C, Murphy et al. 1987)
18.14 (calculated-QSAR-MCI \( \chi \), Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
18.23 (calculated-QSPR, Dunnivant et al. 1992)
Polychlorinated Biphenyls (PCBs) 1739

23.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
\[ \ln K_{AW} = -\Delta H_f / R + \Delta S_f / R; \ R \ is \ the \ ideal \ gas \ constant, \ \Delta H_f = 30 \pm 6 \ \text{kJ/mol}, \ \Delta S_f = 0.07 \pm 0.02 \ \text{kJ/mol-K} \]
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{OW} \):
5.75, 6.67 (RP-HPLC-\( k' \) correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.25, 6.33, 6.35, 6.28 (RP-HPLC-\( k' \) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.31 (recommended, Sangster 1993)
6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
10.49, 9.44 (0, 20°C, multi-column GC-\( k' \) correlation, Zhang et al. 1999)
9.21 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log \( K_B \):
5.43; 6.96 (zebrafish: log BCF \( w \) wet wt basis; log BCF \( l \) lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log \( K_P \) or log \( K_d \):
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Partition Coefficient between particulate and dissolved contaminant concentrations, log \( K_P \) or log \( K_d \):
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log \( K_{OC} \):
6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log \( K_a \), calculated-MCI \( \chi \), Sabljic et al. 1989)
5.83, 5.89, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.69 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.10 (soil-organic carbon, calculated-\( K_{OW} \) Girvin & Scott 1997)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{1/2} \):
Volatilization:
Photolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, *data at other temperatures reference:
\[ k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \]
for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 60–120 \ \text{d}, \) due to gas-phase loss process at room temp. (Atkinson 1987)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
\[ k_1 = 3400 \ \text{d}^{-1}; \ k_2 = 0.0126 \ \text{d}^{-1} \] (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
\[ k_2 = 0.004 \ \text{d}^{-1} \] with \( t_\text{1/2} = 163 \ \text{d} \] (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
\[ k_2 = 0.004 \ \text{d}^{-1} \] with \( t_\text{1/2} = 188 \ \text{d} \] (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 163$ d for high-dose treatment, $t_{1/2} = 188$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Common Name: 2,2′,3,4′,6′-Pentachlorobiphenyl
Synonym: PCB-98
Chemical Name: 2,2′,3,4′,6′-pentachlorobiphenyl
CAS Registry No: 60233-25-2
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
268.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘₙ (kJ/mol):
Entropy of Fusion, ∆Sₘₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₘₙ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0333 (Sᵋ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0153, 0.0116, 0.0124 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.05 × 10⁻³ (Pᵋ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00753, 0.008084 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00615, 0.00751 (supercooled liquid Pᵋ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00692 (supercooled liquid Pᵋ, GC-RI correlation, Fischer et al. 1992)
log (Pᵋ/Pa) = –4399/(T/K) + 12.54 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
68.90 (calculated-P/C, Burkhard 1984)
50.26 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₘₐₜ = –ΔHᵋ/RT + ΔSᵋ/R; R is the ideal gas constant, ΔHᵋ = 18 ± 6 kJ/mol, ΔSᵋ = 0.03 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₒₜₒₜ:
6.36 (calculated-TSA, Burkhard 1984)
5.98, 6.16, 5.99 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.071 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₒₐ:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.16  (suspended particulate matter, Burkhard 1984)
- 4.589  (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 153$ d for high-dose treatment, $t_{1/2} = 164$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.99  2,2′,4,4′,5-Pentachlorobiphenyl (PCB-99)

Common Name: 2,2′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-99, 2,2′,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 38380-01-7
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C): 81.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔHₚ (kJ/mol):
Entropy of Fusion, ΔSₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   0.0353  (supercooled liquid Sₗ, calculated-TSA, Burkhard et al. 1985b)
   0.0222  (20°C, supercooled liquid Sₗ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
   0.00366 (RP-HPLC-k′ correlation, Brodsky & Ballschminter 1988)
   0.0103  (calculated-TSA, Abramowitz & Yalkowsky 1990)
   0.011   (calculated-MCI χ, Patil 1991)
   0.00597 (estimated-EPIWIN v3.04, Hardy 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   0.0029  (supercooled liquid Pₗ, GC-RT correlation, Bidleman 1984)
   0.00735, 0.00342, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
   0.00316 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
   0.00328, 0.00375 (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
   0.00147 (20°C, supercooled liquid Pₗ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
   0.00229 (Pₗ, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
   0.000293 (estimated-EPIWIN v3.04, Hardy 2002)
Henry’s Law Constant (Pa m³/mol at 25°C):
   29.28  (calculated-P/C, Burkhard et al. 1985b)
   21.68  (20°C, calculated-P/C, Murphy et al. 1987)
   30.50  (calculated-QSAR MCI χ, Sabljic & Güsten 1989)
   7.90   (wetted-wall column-GC/ECD, Brunner et al. 1990)
   57.0   (calculated-QSPR, Dunnivant et al. 1992)
   35.4   (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
   51.8   (from 11°C exptl. data and compensation point, Bamford et al. 2002)
   ln KᵦW = − ΔHᵦ/RT + ΔSᵦ/R; R is the ideal gas constant, ΔHᵦ = 16 ± 6 kJ/mol, ΔSᵦ = 0.02 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
- 6.29, 7.21 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 6.41 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
- 6.39 (calculated-TSA, Hawker & Connell 1988a)
- 6.26 (calculated-MCI $\chi$, Patil 1991)
- 6.41 (recommended; Sangster 1993)
- 7.21 (recommended, Hansch et al. 1995)
- 6.60, 6.26–7.21 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
- 6.4014 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 6.9795 (estimated-EPIWIN v3.04, Hardy 2002)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:
- 9.38 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:
- 4.09 (fish, microcosm, Garten & Trabalka 1983)
- 5.14 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$
- 5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.14 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 4.73 (marine humic substance, calculated-MCI $\chi$, reported as log $K_h$ at 5 mg/L DOC, Sabljic et al. 1989)
- 7.00 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.68 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.54 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 6.10 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
- 4.87 (estimated-EPIWIN v3.04, Hardy 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:
Volatilization: $t_\frac{1}{2}$ = 0.6419 d from river, $t_\frac{1}{2}$ = 13.31 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}$(calc) = (0.2–0.4) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}$(calc) = (0.3–0.9) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1$ = 8 (food lipid mg)/(g worm lipid-d); $k_2$ = 0.07 d$^{-1}$ (earthworm, Wågman et al. 2001)
- $k_1$ = 0.003 d$^{-1}$ with $t_\frac{1}{2}$ = 2252 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exppt.- high-dose treatment, Buckman et al. 2004)
- $k_1$ = 0.004 d$^{-1}$ with $t_\frac{1}{2}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exppt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: volatilization $t_{1/2} = 0.6419$ d from river, $t_{1/2} = 13.31$ d from lake (estimated-EPIWIN v.3.04, Hardy 2002).

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 9$ d in earthworm given contaminated food (Wågman et al. 2001)

Depuration $t_{1/2} = 252$ d for high-dose treatment, $t_{1/2} = 172$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment ($8^\circ$C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.100 2,2′,4,4′,6-Pentachlorobiphenyl (PCB-100)

Common Name: 2,2′,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-100, 2,2′,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6-pentachlorobiphenyl
CAS Registry No: 39485-83-1
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C): 95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0275 (supercooled liq., calculated-TSA, Burkhard et al. 1985b)
0.031 (unpublished data of Weil 1978; quoted, Kilzer et al. 1979; Geyer et al. 1980)
0.00666, 0.00580, 0.00941 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.011 (calculated-MCI χ, Patil 1991)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
0.00735, 0.00872, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00818 (supercooled liquid, GC-RT correlation, Burkhard et al. 1985b; quoted, Eisenreich 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
97.27 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
62.62 (calculated-MCI χ, Sabljic & Güsten 1989)
56.98 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = -ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 18 ± 6 kJ/mol, ΔS_{f} = 0.03 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
6.23, 6.37, 6.08 (RP-HPLC-RI correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log K_{OA}:
8.66 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF:
1.11, 1.06 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
0.32 (rodent, Garten & Trabalka 1983)
4.06, 3.91 (algae, calculated, Geyer et al. 1984)
4.06, 3.37, 4.44 (algae, fish, activated sludge, Freitag et al. 1984, 1985; quoted, Halfon & Reggiani 1986)
Polychlorinated Biphenyls (PCBs)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.24 (suspended particulate matter, calculated-$K_OH$, Burkhard 1984)
- 4.567 (marine humic substance, calculated-MCI $\chi$, reported as association coefficient log $K_a$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  \[ k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 60–120 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)} \]
  \[ k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 16–48 \text{ d at room temp. (Kwok et al. 1995)} \]
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  \[ k_2 = 0.010 \text{ d}^{-1} \text{ (10°C, sandworm, Goerke & Ernst 1977; quoted, Waid 1986)} \]

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
7.1.1.101 2,2′,4,5,5′-Pentachlorobiphenyl (PCB-101)

Common Name: 2,2′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-101, 2,2′,4,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 37680-72-3
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C): 78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.2803
Molar Volume (cm³/mol):
- 289.1 (calculated-Le Bas method at normal boiling point)
- 224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
- 18.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
- 53.56 (Miller et al. 1984)
- 53.7, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
- 0.318 (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K, Shiu & Mackay 1986)
- 0.0321 (calculated-\( \Delta S_{\text{fus}} \) and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.031 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
- 0.0103 (shake flask-GC/ECD, Haque & Schmedding 1975; Chiou et al. 1977)
- 0.0042 (generator column-GC/ECD, Weil et al. 1974)
- 0.019 (shake flask-LSC, Metcalf et al. 1975)
- 0.010 (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
- 0.00424 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
- 0.0005; 0.004 (generator column-HPLC/UV; RP-HPLC-RT correlation, Swann et al. 1983)
- 0.0194 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 0.0356 (supercooled liquid Pₐ, calculated-TSA, Burkhard et al. 1985b)
- 0.0154* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
\[
\begin{align*}
\ln x &= -3837/(T/K) - 8.0159, \text{ temp range } 4–32°C, \Delta H_{\text{fus}} = 31.9 \text{ kJ/mol} \quad \text{(generator column-GC/ECD, Dickhut et al. 1986)}
\end{align*}
\]
- log \( x = -1664/(T/K) - 3.478, \Delta H_{\text{fus}} = 31.8 \text{ kJ/mol} \) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
\[
\begin{align*}
S/(\text{mol/L}) &= 1.54 \times 10^{-10} \exp(0.046·T/°C) \quad \text{(regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)}
\end{align*}
\]
- 0.011 (shake flask-GC/ECD, Chiou et al. 1986, 1991)
- 0.0263 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.00402, 0.00517, 0.0070, 0.0070 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
- 0.00674; 0.0222 (generator column-GC/ECD, supercooled liquid \( S_{1} \), Dunnivant & Elzerman 1988)
\[
\begin{align*}
\log [S_{1}/(\text{mol/L})] &= 0.875 - 982.6/(T/K) \quad \text{(supercooled liquid, Passivirta et al. 1999)}
\end{align*}
\]
- In \( x = -8.026 - 3836.44/(T/K) \) (regression eq. of literature data, Shiu & Ma 2000)
Polychlorinated Biphenyls (PCBs)

0.0334 (calculated-mp and K„mp„ Ran et al. 2002)
0.0312, 0.0333 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
\[ \log S_f (\text{mol m}^{-3}) = -1113/(T/K) - 0.27 \] (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0016 (P„s„ from GC-RT correlation, Westcott & Bidleman 1981)
0.000996, 0.001173 (solid P„s„ 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
\[ \log (P/mmHg) = 11.1 - 4840/(T/K); \text{temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)} \]
0.0031 (P„l„ calculated from P„s„ using fugacity ratio F, Westcott & Bidleman 1981)
0.0053, 0.00316 (P„gc„ by GC-RT correlation, different stationary phases, Bidleman 1984)
0.00315 (supercooled liquid P„l„, converted from literature P„s„ with ∆S„f„ Bidleman 1984)
0.00336, 0.00402 (supercooled liquid P„l„, calculated from P„gc„ GC-RT correlation, different stationary phases, Bidleman 1984)
0.00358 (supercooled liquid P„l„, GC-RT correlation, Burkhard 1984, Burkhard et al. 1985b)
0.000225, 0.00118, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00361, 0.00403 (supercooled liquid P„l„, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.000109; 0.0035 (selected solid P„s„; supercooled liquid P„l„, Shiu & Mackay 1986)
0.00142 (20°C, supercooled liquid P„l„, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00359 (supercooled liquid P„l„, Dunnivant & Elzerman 1988)
0.000527; 0.00173 (calculated-S × HLC, solid P„s„; supercooled liquid P„l„, Dunnivant & Elzerman 1988)
\[ \log (P/mmHg) = 11.0 - 4750/(T/K) \] (GC-RT correlation, Tateya et al. 1988)
0.00152 (calculated-UNIFAC group contribution, Banerjee et al. 1990)
0.00315, 0.00296 (supercooled liquid P„l„, converted from literature P„s„ with different ∆S„f„ values, Hinckley et al. 1990)
0.00504, 0.0034 (P„gc„ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
\[ \log (P„l„/Pa) = 12.13 - 4369/(T/K) \] (GC-RT correlation, Hinckley et al. 1990)
0.00257, 0.00398 (supercooled liquid P„l„; GC-RI correlation, different stationary phases, Fischer et al. 1992)
\[ \log (P„l„/Pa) = -4514/(T/K) + 12.67 \] (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
1.33 × 10⁻⁴, 4.16 × 10⁻⁴ (solid, supercooled liquid, Passivirta et al. 1999)
\[ \log (P„l„/Pa) = 15.47 - 5495/(T/K) \] (solid, Passivirta et al. 1999)
\[ \log (P„l„/Pa) = 12.67 - 4514/(T/K) \] (liquid, Passivirta et al. 1999)
\[ (4.04–22.5) × 10⁻⁴; (1.46–40.4) × 10⁻³ \] (literature solid P„s„ range; literature liquid P„l„ range, Delle Site 1997)
0.0020 (supercooled P„l„, calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0024, 0.00245 (supercooled liquid P„l„; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
\[ \log (P„l„/Pa) = -4632/(T/K) + 12.92 \] (supercooled liquid, linear regression of literature data, Li et al. 2003)
\[ \log (P„l„/Pa) = -4346/(T/K) + 11.94 \] (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated † are compiled at the end of this section.):
32.73 (calculated-P/C, Burkhart et al. 1985b)
7.09 (20°C, gas stripping-GC, Oliver 1985)
35.48 (calculated-P/C, Shiu & Mackay 1986)
18.14 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.19 (calculated-QSAR-χ, Sabljic & Güsten 1989)
9.12 (calculated-QSPR, Dunnivant et al. 1992)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
1.424, 4.166 (0, 15°C, from modified two-film model, Hornbuckle et al. 1994)
\[ \log H (\text{Pa m}³/\text{mol}) = 13.55 – 3531/(T/K) \] (Passivirta et al. 1999)
42.07± 0.70 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
\[ \ln K„aw„ = 7.9384 – 3572.29/(T/K); \text{temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)} \]
\[ K„aw„ = \exp[-(29.7/kJ·mol⁻¹) RT + (0.066/kJ·mol⁻¹·K⁻¹)/R]; \text{where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)} \]
\[
\ln K_{AW} = -\Delta H_{H}/RT + \Delta S_{H}/R; \ R \text{ is the ideal gas constant, } \Delta H_{H} = 30 \pm 3 \text{ kJ/mol, } \Delta S_{H} = 0.07 \pm 0.01 \text{ kJ/mol K} \\
\text{(Bamford et al. 2002)—see Comment by Goss et al. 2004)}
\]

31.62, 24.0 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

\[
\log [H/(\text{Pa m}^3/\text{mol})] = -3233/(T/K) + 12.21 \quad \text{(FAV final adjusted eq., Li et al. 2003)}
\]

Octanol/Water Partition Coefficient, \(\log K_{OW}\):

4.12 (radiolabeled-\(^{14}\)C, Metcalf et al. 1975)
6.11 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
7.64 (Hansch & Leo 1979)
6.44 (HPLC-RT correlation, Veith et al. 1979)
6.85 (RP-TLC-k’ correlation, Bruggeman et al. 1982)
6.42 (HPLC-RT correlation, Swann et al. 1983)
5.92 (generator column-GC/ECD, Miller et al. 1984)
6.15, 7.07 (RP-HPLC-k’ correlation, Rapaport & Eisenreich 1984)
7.64 (HPLC-RT correlation, Woodburn et al. 1984)
6.50 (generator column-HPLC, Woodburn et al. 1984)
6.88, 7.0 (HPLC-k’ correlation, calculated, De Kock & Lord 1987)
6.50 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
6.36, 6.39, 6.18, 6.27 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.88 (HPLC-RT correlation, Doucette & Andren 1988)
6.23, 6.18 (RP-HPLC-k’ correlation, different stationary phases, Sherblom & Eganhouse 1988)
6.41 (HPLC-k’ correlation, Noegrohati & Hammers 1992)
6.16 (recommended, Sangster 1993)
6.50 (recommended, Hansch et al. 1995)
6.15, 6.33 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, \(\log K_{OA}\) at 25°C or as indicated and the reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section.

8.30 (calculated-\(K_{OW}/K_{AW}\), Wania & Mackay 1996)
\[
\log K_{OA} = -3.82 + 3841/(T/K); \text{ temp range –10 to 30°C (generator Column-GC, Harner & Bidleman 1996)}
\]

8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

\[
\log K_{OA} = -5.84 + 4360/(T/K) \quad \text{(fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)}
\]

9.79 (10°C, estimated, Thomas et al. 1998)
10.49, 9.44; 9.29 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
9.37 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.14; 9.05 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.90, 8.73 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
\[
\log K_{OA} = 4291/(T/K) - 5.50 \quad \text{(LDV linear regression of literature data, Li et al. 2003)}
\]
\[
\log K_{OA} = 3785/(T/K) - 5.35 \quad \text{(FAV final adjusted eq., Li et al. 2003)}
\]

Bioconcentration Factor, \(\log BCF\):

3.18 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.74, 4.78, 4.08, 4.24 (algae, snail, fish, mosquito, Metcalf et al. 1975)
4.66 (fish, flowing water, Kenaga & Goring; Kenaga 1980)
3.92, 3.60 (calculated-S, calculated-\(K_{OC}\), Kenaga 1980)
4.09 (fish, microcosm, Garten & Trabalka 1983)
3.30–4.15 highest value, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)

> 5.40, 4.15; 6.92 (rainbow trout, laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
2.73, 2.60 (human fat of lipid, wet wt. basis, calculated-\(K_{OW}\), Geyer et al. 1987)
4.15 (fish, quoted, Isnard & Lambert 1988)
Polychlorinated Biphenyls (PCBs)

6.55 (rainbow trout, lipid basis, Noegrohati & Hammers 1992)
5.47; 7.00 (22°C, zebrafish: log BCF$_W$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)
3.32–5.15 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.84–6.26 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.06, 6.06 (Daphnia, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.47, 7.0 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.10, 7.02 (mussel Mytilus edulis: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.03; 3.98 (Oncorhynchus mykiss, wet wt basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$

5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:

4.63 (Kenaga & Goring 1980)
4.74, 4.80 (estimated-S, $K_{OW}$, Lyman 1982)
5.13, 4.67 (estimated-BCF, Lyman 1982)
4.70; 5.45 (soil, slurry method; HPLC-RT correlation, Swann et al. 1983)
6.14 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
5.60; 5.50; 6.60 (field data of sediment trap material; Niagara River-organic matter; calculated-$K_{OW}$, Oliver & Charlton 1984)
5.65 (suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
4.87, 4.07 (Sanhedron soil, Suwannee River, humic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
4.12, 4.10 (Sanhedron soil, Suwannee River, fulvic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
5.1–6.7, 6.2 (suspended sediment, average, Oliver 1987a)
5.41, 5.41, 4.81, 4.01 (Aldrich humic acid Na salt, Fluka-Tridon humic acid, Calcasieu River humic extract, Suwannee River water sample, Sopchoppy River water sample, Chiou et al. 1987)
6.25 (Lake Michigan water column, Swackhamer & Armstrong 1987)

Sorption Partition Coefficient, log $K_{OM}$:

4.77, 4.86, 4.80, 3.86 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log $K_h$, Lara & Ernst 1989)
4.772, 4.726 (marine humic substances of 5 mg/L DOC, reported as association coefficient log $K_h$, quoted exptl; calculated-MCI $\chi$, Sabljic et al. 1984)
5.86 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.58 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.81, 5.83, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.67 (soil, shake flask-GC, Paya-Perez et al. 1991)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.63 (soil, Sabljic et al. 1995)
5.80; 5.58 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
5.90; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.73 (sediment: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)
4.78–7.03; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.59; 6.19, 5.53, 6.04 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log $K_p$:

4.63, 4.84 (quoted, calculated-molecular connectivity indices $\chi$, Sabljic 1984)

Sorption Partition Coefficient, log $K_p$:

4.87–5.35 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)
Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:

Volutilization:
Photolysis: photodegradation rate constants $k = (0.20 \pm 0.01) \text{ h}^{-1}$, $(0.20 \pm 0.04) \text{ h}^{-1}$, with $t_\frac{1}{2} = 3.4 \text{ h}$, $3.7 \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O$ with O$_3$ as or indicated, *data at other temperatures see reference:

$k_{OH}$(calc) = $(0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH(aq.)} = 4.6 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at $25^\circ\text{C}$, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}$(calc) = $(0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate, $k = 1.5 \times 10^{-8} \text{ nmol cell}^{-1} \text{ h}^{-1}$ by species of Alcaligenes and Acinetobacter (Furukawa et al. 1978, selected, NAS 1979);

85% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism Alcaligenes eutrophus H850 (Bedard et al. 1986);

aerobic biodegradation $t_\frac{1}{2}$ = 1.32 d with the addition of polymer chitin, $t_\frac{1}{2}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 180 \text{ d}^{-1}$; $k_2 = 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 0.049 \text{ h}^{-1}$; $k_2 = 0.014 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)

$log(1/k_2) > 3.1$, 3.6 h (fish, quoted, calculated-K$_{OW}$ Hawker & Connell 1988b).

$k_1 = 3850 \text{ d}^{-1}$; $k_2 = 0.0130 \text{ d}^{-1}$ ($22^\circ\text{C}$, zebrafish, 30-d exposure, Fox et al. 1994)

$k_1 = 0.054 \text{ d}^{-1}$ with an elimination $t_\frac{1}{2} = 12.9 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_\frac{1}{2} = 131 \text{ d}$ and $k_2 = 0.012 \text{ d}^{-1}$ with $t_\frac{1}{2} = 56 \text{ d}$ for food concn of 20 ng/g and 148 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 0.00082 \text{ h}^{-1}$; $k_2 = 0.160 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1$(calc) = 6 (food lipid mg)/(g worm lipid-d); $k_2$(calc) = 0.06 d$^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_\frac{1}{2} = 172 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_\frac{1}{2} = 246 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995);

suggested $t_\frac{1}{2} = 3000 \text{ h}$ at $7^\circ\text{C}$ for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: aerobic biodegradation $t_\frac{1}{2}$ = 1.32 d with the addition of polymer chitin, $t_\frac{1}{2}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted. Abramowicz 1990);

half-lives range from $t_\frac{1}{2}$ ~ 4–11 d in freshwater systems, $t_\frac{1}{2}$ = 0.1–10 d in cloud water, $t_\frac{1}{2}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
photodegradation \( t_{1/2} = (3.4 \pm 0.15) \text{ h}, (3.7 \pm 0.8) \text{ h} \) in aqueous solution with the presence of diethy-lamine after exposure to simulated sunlight (Lin et al. 1995); 
\( t_{1/2} = 60000 \text{ h at } 7^\circ\text{C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \)

**Groundwater:**
Sediment: \( t_{1/2} = 87600 \text{ h at } 7^\circ\text{C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \)

**Soil:** Sorption-Desorption Rate Constants: release rate constants \( k_d \) for labile PCBs sorbed to utility substation soils are: \( k = 0.039 \text{ d}^{-1} \) from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, \( k = 0.65 \text{ d}^{-1} \) from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, \( k = 0.54 \text{ d}^{-1} \) from Tarehee surface soil consist of sand and silt with 0.02% OC and \( k = 0.24 \text{ d}^{-1} \) from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants \( k_d \) for nonlabile PCBs sorbed to utility substation soils are \( k = 0.00064 \text{ d}^{-1} \) from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, \( k = 0.00188 \text{ d}^{-1} \) from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, \( k = 0.00073 \text{ d}^{-1} \) from Tarehee surface soil consist of sand and silt with 0.02% OC and \( k = 0.00247 \text{ d}^{-1} \) from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

\( t_{1/2} = 87600 \text{ h at } 7^\circ\text{C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \)

**Biota:** \( t_{1/2} = 1000 \text{ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and } t_{1/2} = 85 \text{ d in its muscle, (Niimi & Oliver 1983);} \)

elimination \( t_{1/2} = 12.9 \text{ from earthworm (Belfroid et al. 1995)} \)

depuration \( t_{1/2} = 56–131 \text{ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)} \)

\( t_{1/2} = 4.3 \text{ h in blood plasma (ring doves, Drouillard & Norstrom 2000);} \)

depuration \( t_{1/2} = 12 \text{ d in earthworm given contaminated food (predicted, Wågman et al. 2001).} \)

depuration \( t_{1/2} = 172 \text{ d for high-dose treatment, } t_{1/2} = 24446 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)} \)

---

**TABLE 7.1.1.101.1**

Reported aqueous solubilities, vapor pressures, Henry’s law constants and octanol-air partition coefficients of 2,2’,4,5,5’-pentachlorobiphenyl (PCB-101) at various temperatures and the reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
<th>log ( K_{OA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC</td>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>( t/°\text{C} )</td>
<td>( S/\text{g}·\text{m}^{-3} )</td>
<td>( t/°\text{C} )</td>
<td>( P/\text{Pa} )</td>
</tr>
<tr>
<td>4</td>
<td>0.0061</td>
<td>25</td>
<td>0.00096</td>
</tr>
<tr>
<td>20</td>
<td>0.0121</td>
<td>30</td>
<td>0.00173</td>
</tr>
<tr>
<td>25</td>
<td>0.0154</td>
<td></td>
<td>18</td>
</tr>
<tr>
<td>32</td>
<td>0.0223</td>
<td></td>
<td>25</td>
</tr>
<tr>
<td>log ( P/\text{mmHg} = A – B/(T/K) )</td>
<td>A</td>
<td>11.1</td>
<td>( \ln K_{OA} = –\Delta H/\text{RT} + \Delta S/R )</td>
</tr>
<tr>
<td>( \ln x = A – B/(T/K) )</td>
<td>A</td>
<td>( 11.1 )</td>
<td></td>
</tr>
<tr>
<td>4–32°C</td>
<td></td>
<td>B</td>
<td>4840</td>
</tr>
<tr>
<td>( \Delta H_{\text{sol}}/(\text{kJ}·\text{mol}^{-1}) = 31.9 ± 1.9 )</td>
<td>temp range 30–40°C</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 7.1.1.101.1 Logarithm of mole fraction solubility, vapor pressure, Henry’s law constant and \( K_{OA} \) versus reciprocal temperature for \( 2,2',4,5,5' \)-pentachlorobiphenyl (PCB-101).
7.1.1.102 2,2',4,5,6'-Pentachlorobiphenyl (PCB-102)

Common Name: 2,2',4,5,6'-Pentachlorobiphenyl
Synonym: PCB-102, 2,2',4,5,6'-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',4,5,6'-pentachlorobiphenyl
CAS Registry No: 68194-06-9
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C): 93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0314 (Sₜ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0065 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.61 × 10⁻³ (P_L, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00706, 0.00184 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
0.00527, 0.00667 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 10.80 – 4630/(T/K) (GC-RT correlation, Tateya et al. 1988)
log (P_L/Pa) = – 4399/(T/K) + 12.48 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
68.60 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
37.6 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ΔH_m/RT + ΔS_m/R; R is the ideal gas constant, ΔH_m = 18 ± 6 kJ/mol, ΔS_m = 0.03 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
6.39 (calculated-TSA, Burkhard 1984)
6.0959 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
9.13 (calculated-QSPR/quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{bi}:
Sorption Partition Coefficient, log K_{OC}:

- 6.19 (suspended particulate matter, Burkhard 1984)
- 4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_{a}, calculated-MCI \( \chi \), Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, \( t_{\frac{1}{2}} \):

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_{3} radical and \( k_{O3} \) with O_{3} or as indicated, *data at other temperatures see reference:

\[ k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 60–120 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)

\[ k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 16–48 \text{ d} \) at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
Polychlorinated Biphenyls (PCBs)

7.1.1.103 2,2',4,5',6-Pentachlorobiphenyl (PCB-103)

Common Name: 2,2',4,5',6-Pentachlorobiphenyl
Synonym: PCB-103, 2,2',4,5',6-pentachloro-1,1'-biphenyl
Chemical Name: 2,2',4,5',6-pentachlorobiphenyl
CAS Registry No: 60145-21-3
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433

Melting Point (°C): 81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₜₚ (kJ/mol):
Entropy of Fusion, ΔSₜₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₚ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0275 (S₄ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00986, 0.00843, 0.0164, 0.0113 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.23 × 10⁻³ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00983, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00887, 0.0112 (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00617 (supercooled liquid Pₗ: GC-RI correlation, Fischer et al. 1992)
log (Pₗ/Pa) = – 4399/(T/K) + 12.70 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
109.43 (calculated-P/C, Burkhard 1984)
56.24 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.02 (calculated-QSPR, Dunivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₜₚₗ = – ΔHₜₚₗ/RT + ΔSₜₚₗ/R; R is the ideal gas constant, ΔHₜₚₗ = 18 ± 6 kJ/mol, ΔSₜₚₗ = 0.03 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log Kₕₜₚₗ:
6.44 (calculated-TSA, Burkhard 1984)
6.11, 6.25, 5.92, 6.14 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.11 (recommended, Sangster 1993)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.1499 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{B}$:

Sorption Partition Coefficient, log $K_{OC}$:
6.24 (suspended particulate matter, Burkhard 1984)
4.567 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{b}$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.104 2,2′,4,6,6′-Pentachlorobiphenyl (PCB-104)

Common Name: 2,2′,4,6,6′-Pentachlorobiphenyl
Synonym: PCB-104, 2,2′,4,6,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,6,6′-pentachlorobiphenyl
CAS Registry No: 56558-16-8
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
85.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 0.258 (mp at 85°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.030 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0156 (generator column-GC, Dunnivant & Elzerman 1988)
0.0411 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00986 (calculated-group contribution method, Kühne et al. 1995)
0.00651, 0.0175 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0666 (calculated-mp and K_{OW}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C):
0.017 (supercooled liquid P_L, Burkhard 1984)
0.00735, 0.018, 0.00419 (supercooled liquid P_L, calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985a)
0.0170 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00434 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
0.00434 (calculated-S × HLC, solid P_S, Dunnivant & Elzerman 1988)
0.00225 (P_L, calculated-MCI \( \beta \chi \) and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
185.4 (calculated-P/C, Burkhard et al. 1985b)
90.9 (gas stripping, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
55.4 (calculated-QSAR-MCI \( \chi \), Sabljić & Güsten 1989)
75.11 (calculated-QSPR, Dunnivant et al. 1992)
39.40, 47.17, 56.0, 66.0± 1.4, 75.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
\( \ln K_{AW} = 2.1650 - 1774.05/(T/K); \) temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
\( K_{AW} = \exp[-(14.5/kJ·mol⁻¹)/RT] + (0.018/kJ·mol⁻¹·K⁻¹)/R]; \) where \( R = 8.314 \) J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
62.0 (exptl. data, Bamford et al. 2002)
\( \ln K_{AW} = -\Delta H_f/RT + \Delta S_f/R; \) R is the ideal gas constant, \( \Delta H_f = 15 ± 3 \) kJ/mol, \( \Delta S_f = 0.02 ± 0.01 \) kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

© 2006 by Taylor & Francis Group, LLC
Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 6.40 (calculated-TSA, Burkhard 1984)
- 5.37 (generator column-GC, Hawker & Connell 1988a; quoted, Sangster 1993)
- 5.81 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 6.61 (calculated-Characteristic Root Index CRI, Saçan & Inel 1995)
- 5.7636 (calculated-molecular properties MNDO-AM1, Makino 1998)
- 5.96 (calculated-QSPR, Yeh & Hong 2002)
- 6.59 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

- 8.46 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

- 6.20 (suspended particulate matter, calculated-$K_{ow}$, Burkhard 1984)
- 4.431 (marine humic substances, reported as association coefficient $\log K_h$ at 5 mg L$^{-1}$ DOC, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_2 > 0.0007$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 6$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.10$ d$^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} > 1000$ d in rainbow trout, and $t_{1/2} = 101$ d in its muscle (Niimi & Oliver 1983);

elimination $t_{1/2} = 7$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.105 2,3',4,4'-Pentachlorobiphenyl (PCB-105)

Common Name: 2,3',4,4'-Pentachlorobiphenyl
Synonym: PCB-105, 2,3',4,4'-pentachloro-1,1'-biphenyl
Chemical Name: 2,3',4,4'-pentachlorobiphenyl
CAS Registry No: 32598-14-4
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
103 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C, assuming $\Delta S_{\text{fus}} = 56$ J/mol K, F: 0.164 (at mp 103°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0405 (S, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00236, 0.0119, 0.00636, 0.00517 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)
0.000982, 0.00190 (generator column-GC/ECD, estimated, Hong & Qiao 1995)
0.00166* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.0362, 0.08243 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log $[S]_{\text{L}}/(\text{mol m}^{-3})$ = – 1285/(T/K) + 0.18 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.7 × 10^{-4}, 9.35 × 10^{-4} (supercooled liquid $P_L$ by GC-RT correlation, different stationary phases, Bidleman 1984)
7.07 × 10^{-4} (P$_L$ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00124, 0.000132, 0.000233 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)
8.85 × 10^{-4}, 6.77 × 10^{-4} (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62 × 10^{-4}, 7.76 × 10^{-4} (supercooled liquid $P_L$, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log $(P_L/P_a) = -4758/(T/K) + 12.90$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
2.54 × 10^{-3} ($P_L$, calculated-MCI $\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)
8.71 × 10^{-4}, 1.23 × 10^{-3} (supercooled liquid $P_L$; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log $P_L/P_a = -4554/(T/K) + 12.29$ (supercooled liquid $P_L$, FAV final adjusted eq., Li et al. 2003)

Henry’s Law Constant (Pa-m₃/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
5.68 (calculated-P/C, Burkhard 1985a)
6.08 (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
10.06 (calculated-QSPR, Dunnivant et al. 1992)
2.43 (calculated-QSPR, Achman et al. 1993)
ln $K_{NW} = 26.221 - 9093.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

$K_{NW} = \exp[-(75.6/kJ\cdot mol^{-1})/RT] \times (0.218/kJ\cdot mol^{-1}\cdot K^{-1}/R]$; where $R = 8.314 J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

33.9 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_{m}/RT + \Delta S_{m}/R$; $R$ is the ideal gas constant, $\Delta H_{m} = 76 \pm 8$ kJ/mol, $\Delta S_{m} = 0.22 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

33.88, 13.80 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log H/(Pa\ m^{3}/mol) = -3269/(T/K) + 12.1$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $log K_{OW}$:

6.41, 6.68, 7.14, 6.93 (RP-HPLC-k corr. correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.82 (generator column-GC; Hawker & Connell 1988a)

6.79 (recommended, Sangster 1993)

6.65 (recommended, Hansch et al. 1995)

4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

6.61 (generator column-GC/ECD, Yeh & Hong 2002)

6.61, 6.82 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

10.27* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)

$\log K_{OA} = -5.68 + 4678/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)

11.41, 10.20; 10.02 (0, 20°C, multi-column GC-k corr. correlation; calculated at 20°C, Zhang et al. 1999)

10.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4630/(T/K) - 6.0$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $log BCF$ or $log K_{B}$:

2.82–4.26 (various marine species, mean dry weight, Hope et al. 1998)

Sorption Partition Coefficient, $log K_{OC}$:

6.09 (suspended particulate matter, calculated-K ow, Burkhard 1984)

4.906 (as log $K_{h}$ association coefficient with marine humic substance, calculated-MCI $\chi$, Sabljic et al. 1989)

5.81 (soil, shake flask-GC, Paya-Perez et al. 1991)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \ cm^{3} \ molecule^{-1} \ s^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \ cm^{3} \ molecule^{-1} \ s^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_{1}$ and $k_{2}$):
k₂ = 0.014 d⁻¹ with t½ = 48 d and k₂ = 0.014 d⁻¹ with t½ = 50 d for food concn of 17 ng/g and 133 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k₂ = 0.004 d⁻¹ with t½ = 181 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)

k₂ = 0.003 d⁻¹ with t½ = 204 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: t½ = 7 yr (Geyer et al. 2000)

Soil:

Biota: reported biological t½ = 155 to > 1000 d for trout, t½ = 62–101 d for trout muscle; t½ = 73 to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)

Depuration t½ = 49–50 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration t½ = 181 d for high-dose treatment, t½ = 204 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

**TABLE 7.1.1.105.1**

Reported aqueous solubilities, Henry’s law constants and octanol-air partition coefficients of 2,3,3′,4,4′-pentachlorobiphenyl (PCB 105) at various temperatures and reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry’s law constant</th>
<th>log KOA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Huang &amp; Hong 2002</td>
<td>Bamford et al. 2000</td>
<td>Harner &amp; Bidleman 1996</td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
</tr>
<tr>
<td>5</td>
<td>5.58 × 10⁻⁴</td>
<td>4</td>
</tr>
<tr>
<td>15</td>
<td>8.89 × 10⁻⁴</td>
<td>11</td>
</tr>
<tr>
<td>25</td>
<td>1.66 × 10⁻³</td>
<td>18</td>
</tr>
<tr>
<td>35</td>
<td>2.98 × 10⁻³</td>
<td>25</td>
</tr>
</tbody>
</table>

ln x = A – B/(T/K)
mole fraction x

ln KAW = −ΔH/RT + ΔS/R

A
B
ΔHsol/R

A
B
9093.1

mp/°C | 116.5–117.5
ΔHsol/(kJ mol⁻¹) = 40.1

enthalpy, entropy change:

ΔH/(kJ mol⁻¹) = 75.6 ± 8.4

ΔS/(J·mol⁻¹·K⁻¹) = 218 ± 28

© 2006 by Taylor & Francis Group, LLC
FIGURE 7.1.1.105.1 Logarithm of mole fraction solubility, Henry's law constant and $K_{OA}$ versus reciprocal temperature for 2,3,3′,4,4′-pentachlorobiphenyl (PCB-105).
### 7.1.1.106 2,3,3′,4,5-Pentachlorobiphenyl (PCB-106)

![Chemical Structure](image)

**Common Name:** 2,3,3′,4,5-Pentachlorobiphenyl  
**Synonym:** PCB-106, 2,3,3′,4,5-pentachloro-1,1′-biphenyl  
**Chemical Name:** 2,3,3′,4,5-pentachlorobiphenyl  
**CAS Registry No:** 70424-69-0  
**Molecular Formula:** C_{12}H_{5}Cl_{5}  
**Molecular Weight:** 326.433  
**Melting Point (°C):** 105 (estimated, Abramowitz & Yalkowsky 1990)  
**Boiling Point:**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 289.1 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):**  
**Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), F:**  

**Water Solubility (g/m³ or mg/L at 25°C):**  
0.0411 (Sₜ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.0082, 0.0088, 0.00517, 0.0058 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
0.0050 (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00735, 0.0180, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985b)  
0.00138, 0.00127 (supercooled liquid \( P_{1} \), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  

\[ \log (P_1/P_a) = -4688/(T/K) + 12.86 \]  

**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
39.82 (calculated-P/C, Burkhard 1984)  
19.66 (calculated-QSPR-MCI \( \chi \), Sabljic & Güsten 1989)  
16.7 (calculated-QSPR, Dunnivant et al. 1992)  
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  

\[ \ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; R \text{ is the ideal gas constant, } \Delta H_{f} = 56 \pm 17 \text{ kJ/mol, } \Delta S_{f} = 0.15 \pm 0.01 \text{ kJ/mol-K} \]  

**Octanol/Water Partition Coefficient, log \( K_{ow} \):**  
6.29 (calculated-TSA, Burkhard 1984)  
6.79, 6.79, 7.22, 6.89 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
6.64 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)  
6.92 (recommended, Sangster 1993)  
6.6213 (calculated-molecular properties MNDO-AMI method, Makino 1998)  

**Octanol/Air Partition Coefficient, log \( K_{oa} \):**  
9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{bc}:

Sorption Partition Coefficient, log K_{OC}:

- 6.09 (suspended particulate matter, Burkhard 1984)
- 4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_{as}, calculated-MCI \chi, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

- k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau_{(calc)} = 60–120 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}
- k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } \tau_{(calc)} = 16–48 \text{ d at room temp. (Kwok et al. 1995)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
Polychlorinated Biphenyls (PCBs)

7.1.1.107 2,3′,4′,5-Pentachlorobiphenyl (PCB-107)

Common Name: 2,3′,4′,5-Pentachlorobiphenyl
Synonym: PCB-107, 2,3′,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4′,5-pentachlorobiphenyl
CAS Registry No: 70424-68-9
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
105 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH₉₀ (kJ/mol):
Entergy of Fusion, ΔS₉₀ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉₀ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0359 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0148 (20°C, supercooled liquid, Murphy et al. 1987)
0.0026 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00105 (Pₗ supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00116, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
2.61 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
0.00105, 0.00132 (supercooled liquid Pₗ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₗ/Pₕ) = – 4688/(T/K) + 12.82 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
9.63 (calculated-P/C, Burkhard 1984)
8.61 (20°C, calculated-P/C, Murphy et al. 1987)
20.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
16.13 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
16.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln Kₜₙₜ = – ΔHᵣ/R + ΔSᵣ/R; R is the ideal gas constant, ΔHᵣ = 43 ± 7 kJ/mol, ΔSᵣ = 0.11 ± 0.02 kJ/mol-K
Octanol/Water Partition Coefficient, log Kₜₙₜ:
6.34 (calculated-P/C, Burkhard 1984)
6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.5952 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₜₜₛ:
9.58 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log Kₕ:
Sorption Partition Coefficient, log $K_{OC}$:
- 6.14 (suspended particulate matter, Burkhard 1984)
- 4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatile:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ as indicated, *data at other temperatures see reference:
- $k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_2 = 0.004$ d$^{-1}$ with $t_\frac{1}{2} = 194$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.002$ d$^{-1}$ with $t_\frac{1}{2} = 283$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_\frac{1}{2} = 194$ d for high-dose treatment, $t_\frac{1}{2} = 283$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.108 2,3,3’,4,5’-Pentachlorobiphenyl (PCB-108)

Common Name: 2,3,3’,4,5’-Pentachlorobiphenyl
Synonym: PCB-108, 2,3,3’,4,5’-pentachloro-1,1’-biphenyl
Chemical Name: 2,3,3’,4,5’-pentachlorobiphenyl
CAS Registry No: 70362-41-3
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
73  (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0356  (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0153  (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.00517  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00103  (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00115, 0.000352  (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)
0.00142, 0.00118  (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00105  (supercooled liquid Pₗ, GC-RI correlation, Fischer et al. 1992)
$log (P_{L}/Pa) = -4688/(T/K) + 12.87$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
9.57  (calculated-P/C, Burkhard 1984)
35.26  (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
17.81  (calculated-QSPR, Dunnivant et al. 1992)
36.7  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$log K_{AW} = -\Delta H_{f\text{fus}}/RT + \Delta S_{f\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{f\text{fus}} = 56 \pm 7$ kJ/mol, $\Delta S_{f\text{fus}} = 0.15 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{ow}$:
6.34  (calculated-TSA, Burkhard 1984)
6.57  (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
6.71  (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6672  (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{oa}$:
9.86  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_{b}$:
Sorption Partition Coefficient, log $K_{OC}$:
6.14 (suspended particulate matter, Burkhard 1984)
4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.109 2,3,3',4,6-Pentachlorobiphenyl (PCB-109)

![Chemical structure of 2,3,3',4,6-Pentachlorobiphenyl (PCB-109)](image)

**Common Name:** 2,3,3',4,6-Pentachlorobiphenyl  
**Synonym:** PCB-109, 2,3,3',4,6-pentachloro-1,1'-biphenyl  
**Chemical Name:** 2,3,3',4,6-pentachlorobiphenyl

**CAS Registry No:** 74472-35-8  
**Molecular Formula:** C₁₂H₅Cl₅  
**Molecular Weight:** 326.433

- **Melting Point (°C):** 73 (estimated, Abramowitz & Yalkowsky 1990)
- **Boiling Point (°C):**
- **Density (g/cm³):**
- **Molar Volume (cm³/mol):** 289.1 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):**
- **Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):**
- **Fugacity Ratio at 25°C (assuming $\Delta S_{ fus} = 56$ J/mol K), $F$:**

**Water Solubility (g/m³ or mg/L at 25°C):**
- 0.0434 (S₈, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

**Vapor Pressure (Pa at 25°C):**
- 0.0063 (P₈, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 0.00735, 0.00675, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)

**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):**
- 47.52 (calculated-P/C, Burkhard 1984)
- 28.56 (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
- 39.42 (calculated-QSPR, Dunnivant et al. 1992)
- 44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[
\ln K_{AW} = -\Delta H_{H} / R + \Delta S_{H} / R; \text{ R is the ideal gas constant, } \Delta H_{H} = 29 \pm 8 \text{ kJ/mol, } \Delta S_{H} = 0.06 \pm 0.01 \text{ kJ/mol·K} \\
(\text{Bamford et al. 2002)—see Comment by Goss et al. 2004})
\]

**Octanol/Water Partition Coefficient, log $K_{OW}$:**
- 6.27 (calculated-TSA, Burkhard 1984)
- 6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.5063 (quoted expvl., calculated-molecular properties MNDO-AM1 method, Makino 1998)

**Octanol/Air Partition Coefficient, log $K_{OA}$:**
- 9.59 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

**Bioconcentration Factor, log $BCF$ or log $K_{B}$:**

**Sorption Partition Coefficient, log $K_{OC}$:**
- 6.07 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{h}$, calculated-MCI $\chi$, Sabljic et al. 1989)
Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:

\[ k_{\text{OH}}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 60–120 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)

\[ k_{\text{OH}}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 16–48 \text{ d} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k1 and k2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.110 2,3,3’,4’,6-Pentachlorobiphenyl (PCB-110)

Common Name: 2,3,3’,4’,6-Pentachlorobiphenyl
Synonym: PCB-110, 2,3,3’,4’,6-pentachloro-1,1’-biphenyl
Chemical Name: 2,3,3’,4’,6-pentachlorobiphenyl
CAS Registry No: 38380-03-9
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
79 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0434 (supercooled liquid S₁, calculated-TSA, Burkhard et al. 1985b)
0.0288 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00731 (RP-HPLC-k’ correlation, Brodsky & Bailes 1988)
0.0082 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI \( \chi \), Patil 1991)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00735, 0.00248, 0.000804(calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985a)
0.00228 (supercooled liquid P₁, GC-RI correlation, Burkhard et al. 1985b)
0.00182, 0.00199(supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.48 \times 10^{-4} (20°C, supercooled liquid P₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
\log (P/mmHg) = 11.0 - 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00141, 0.00224 (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)
\log (P₁/Pa) = -4522/(T/K) + 12.43 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.00258 (P₁, calculated-MCI \( \chi \) and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
37.48 (calculated-P/C, Murphy et al. 1983)
17.12 (calculated-P/C, Burkhard et al. 1985b)
10.74 (20°C, calculated-P/C, Murphy et al. 1987)
19.15 (calculated-QSPR-MCI \( \chi \), Sabljic & Güsten 1989)
19.89 (calculated-QSPR, Dunnivant et al. 1992)
5.966 (calculated-QSPR, Achman et al. 1993)
18.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
\ln K_{\text{AW}} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R; \ R \ is \ the \ ideal \ gas \ constant, \ \Delta H_{\text{f}} = 38 \pm 7 \ \text{kJ/mol}, \ \Delta S_{\text{f}} = 0.09 \pm 0.02 \ \text{kJ/mol-K} \ (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 6.20 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
- 6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.22 (generator column-GC, Larsen et al. 1992)
- 6.20 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log $K_{OA}$ or as indicated and reported temperature dependence equations:

- 9.06; 8.58 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.16 + 4540/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 10.14 (10°C, estimated, Thomas et al. 1998)
- 9.06 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
- 10.61, 9.80; 9.80 (0, 20°C, multi-column GC-'k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 9.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 5.18, 6.48 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_p$ or log $K_d$

- 5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.50 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.06 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.6–6.8, 6.4; 7.70(suspended sediment, average; algae > 50μm, Oliver 1987a)
- 4.72, 4.80, 4.77, 3.79 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_p$, Lara & Ernst 1989)
- 4.72, 4.75 (marine humic substances of 5 mg/L DOC, quoted, calculated-MCI χ, Sabljic et al. 1989)
- 6.32 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.20 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.71 (soil, shake flask-GC, Paya-Perez et al. 1991)
- 6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
- 5.80 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation rate constant $k = (0.07 ± 0.01) h^{-1}$ with $t_{1/2} = 9.9$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(aq.) = 4.3 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton’s reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} = 4–11$ d in freshwater systems, $t_{1/2} = 0.1–10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:
Polychlorinated Biphenyls (PCBs)

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 0.00064 \text{ h}^{-1}$; $k_2 = 0.094 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 204 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water: half-lives range from $t_{1/2} \sim 4–11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1–10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991); photodegradation $t_{1/2} = (9.9 \pm 1.6) \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

- Groundwater:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 171 \text{ d}$ for high-dose treatment, $t_{1/2} = 204 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment ($8^\circ\text{C}$, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.111 2,3,3',5,5'-Pentachlorobiphenyl (PCB-111)

Common Name: 2,3,3',5,5'-Pentachlorobiphenyl
Synonym: PCB-111, 2,3,3',5,5'-pentachlоро-1,1'-biphenyl
Chemical Name: 2,3,3',5,5'-pentachlorobiphenyl
CAS Registry No: 39635-32-0
Molecular Formula: C\textsubscript{12}H\textsubscript{5}Cl\textsubscript{5}
Molecular Weight: 326.433

Melting Point (°C):
79 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm\textsuperscript{3}):

Molar Volume (cm\textsuperscript{3}/mol):
289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta H\text{_{ fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S\text{_{ fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S\text{_{ fus}} = 56$ J/mol K), $F$:

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
0.0315 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00156 (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)

Henry’s Law Constant (Pa-m\textsuperscript{3}/mol at 25°C):
16.21 (calculated-P/C, Burkhard 1984)
49.45 (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
19.89 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = - \frac{\Delta H_{H}/RT + \Delta S_{H}/R}{R}$; $R$ is the ideal gas constant, $\Delta H_{H} = 56 \pm 17$ kJ/mol, $\Delta S_{H} = 0.15 \pm 0.01$ kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{OW}$:
6.39 (calculated-TSA, Burkhard 1984)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.7224 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{OA}$:
10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$ or log $K_{B}$:

Sorption Partition Coefficient, log $K_{OC}$:
6.19 (suspended particulate matter, Burkhard 1984)
4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{a}$, calculated-MCI $\chi$, Sabljic et al. 1989)
Polychlorinated Biphenyls (PCBs)

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volutilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } t(\text{calc}) = 60–120 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)}

k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for pentachlorobiphenyls, and the tropospheric lifetime } t(\text{calc}) = 16–48 \text{ d at room temp. (Kwok et al. 1995)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
### 7.1.1.112 2,3,3′,5,6-Pentachlorobiphenyl (PCB-112)

![Chemical Structure](image)

**Common Name:** 2,3,3′,5,6-Pentachlorobiphenyl  
**Synonym:** PCB-112, 2,3,3′,5,6-pentachloro-1,1′-biphenyl  
**Chemical Name:** 2,3,3′,5,6-pentachlorobiphenyl  
**CAS Registry No:** 74472-36-9  
**Molecular Formula:** C_{12}H_{5}Cl_{5}  
**Molecular Weight:** 326.433  
**Melting Point (°C):** 65 (estimated, Abramowitz & Yalkowsky 1990)  
**Boiling Point (°C):**  
**Density (g/cm³):** 289.1 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):**  
**Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), \( F \):**  
**Water Solubility (g/m³ or mg/L at 25°C):**  
0.0463 (\( S_L \) supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00382, 0.00783, 0.00430, 0.00765 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
5.91 × 10⁻³ (\( P_L \) supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)  
0.00316 (supercooled liquid \( P_L \), GC-RI correlation, Fischer et al. 1992)  
\[ \log (P_L/P_a) = -4522/(T/K) + 12.65 \] (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
41.75 (calculated-P/C, Burkhard 1984)  
33.34 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)  
27.02 (calculated-QSPR, Dunnivant et al. 1992)  
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\[ \ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R; \ R \text{ is the ideal gas constant, } \Delta H_{\text{fus}} = 29 \pm 8 \text{ kJ/mol, } \Delta S_{\text{fus}} = 0.06 \pm 0.01 \text{ kJ/mol·K} \] (Bamford et al. 2002)—see Comment by Goss et al. 2004  
**Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):**  
6.24 (calculated-TSA, Burkhard 1984)  
6.40, 6.28, 6.70, 6.25 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
6.45 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)  
6.41 (recommended, Sangster 1993)  
6.4916 (calculated-molecular properties MNDO-AM1 method, Makino 1998)  
**Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):**  
9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_b:

Sorption Partition Coefficient, log K_OC:

- 6.04 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI 1/χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 as indicated, *data at other temperatures see reference:

\[ k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 60–120 \text{ d, due to gas-phase loss process at room temp. (Atkinson 1987)} \)

\[ k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(\text{calc}) = 16–48 \text{ d at room temp. (Kwok et al. 1995)} \)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

\[ k_1 = 12 \text{ (food lipid mg)/(g worm lipid-d); k_2 = 0.06 d}^{-1} \text{ (earthworm, Wågman et al. 2001)} \]

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination t½ = 11 d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.113 2,3,3′,5′,6-Pentachlorobiphenyl (PCB-113)

Common Name: 2,3,3′,5′,6-Pentachlorobiphenyl
Synonym: PCB-113, 2,3,3′,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5′,6-pentachlorobiphenyl
CAS Registry No: 68194-10-5
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
65 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0382 (S, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0036 (RP-HPLC-k correlation, Brodsky & Ballschmitter 1988)
0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.372 × 10⁻³ (P, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00365, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00306, 0.00368 (supercooled liquid P,, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00240 (supercooled liquid P,, GC-RI correlation, Fischer et al. 1992)
log (P/Pa) = – 4522/(T/K) + 12.63 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
28.88 (calculated-P/C, Burkhard 1984)
48.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ∆H_{f}/RT + ∆S_{f}/R; R is the ideal gas constant, ∆H_{f} = 29 ± 8 kJ/mol, ∆S_{f} = 0.06 ± 0.01 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k correlation, Brodsky & Ballschmitter 1988)
6.54 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.45 (recommended, Sangster 1993)
6.3808 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
9.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

6.11 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: measured rate constant $k < 0.05 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.3 and $23 \pm 2 ^\circ \text{C}$, with $t_{1/2} > 8 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil:

Biota:
7.1.1.114 2,3,4,4′,5-Pentachlorobiphenyl (PCB-114)

![Chemical Structure of 2,3,4,4′,5-Pentachlorobiphenyl](image)

Common Name: 2,3,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-114, 2,3,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,5-pentachlorobiphenyl
CAS Registry No: 74472-37-0
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433

Melting Point (°C):
- 99 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
- 109 (Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³):
- 289.1 (calculated-Le Bas method at normal boiling point)
- 224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ∆Hₚₜ (kJ/mol):

Entropy of Fusion, ∆Sₚₜ (J/mol K):

Fugacity Ratio at 25°C (assuming ∆Sₚₜ = 56 J/mol K), F: 0.188 (at mp 99°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
- 0.0121, 0.00879 (RP-HPLC-k’ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
- 0.00146; 0.00246 (generator column-GC/ECD; estimated, Hong & Qiao 1995)
- 0.00263 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
- 0.000732, 0.00157, 0.00263, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 5.58 × 10⁻³ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 0.00136, 0.000881, 0.000352 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
- 3.45 × 10⁻⁴ (20°C, supercooled liquid P₁, Murphy et al. 1987)
- 0.00124, 0.000115 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 6.92 × 10⁻⁴ (supercooled liquid P₁; GC-RI correlation, Fischer et al. 1992)
- log (P₁/Pa) = –4688/(T/K) + 12.82 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 42.56 (calculated-P/C, Burkhard et al. 1985a)
- 6.99 (20°C, calcd-P/C, Murphy et al. 1987)
- 14.48 (calculated-QSPR, Dunnivant et al. 1992)
- 4.96 (calculated-QSPR, Achman et al. 1993)
- 36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln K₆ₗ = –ΔHᵢ'/RT + ΔSᵢ'/R; R is the ideal gas constant, ΔHᵢ' = 56 ± 17 kJ/mol, ΔSᵢ' = 0.15 ± 0.01 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log Kₖₖₗ:
- 6.29 (calculated-TSA, Burkhard 1984)
Polychlorinated Biphenyls (PCBs) 1783

6.45, 6.78 (RP-HPLC-k correlation, different mobile phases, Brodsky & Ballschmiter 1988)
6.65 (calculated, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.72 (recommended, Sangster 1993)
6.5879 (calculated-molecular properties MNDO-AM1, Makino 1998)
6.47 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$:
9.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
5.34, 6.65 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
6.09 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
4.906 (as log $K_a$ association coefficient with marine humic substance, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_1/2$:
Vaporization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $t(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $t(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Biocenclation and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 187$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota: reported biological $t_{1/2} = 155$ to > 1000 d for trout, $t_{1/2} = 62–101$ d for trout muscle; $t_{1/2} = 73$ to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)
depuration $t_{1/2} = 164$ d for high-dose treatment, $t_{1/2} = 187$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.115 2,3,4,4’,6-Pentachlorobiphenyl (PCB-115)

Common Name: 2,3,4,4’,6-Pentachlorobiphenyl
Synonym: PCB-115, 2,3,4,4’,6-pentachloro-1,1’-biphenyl
Chemical Name: 2,3,4,4’,6-pentachlorobiphenyl
CAS Registry No: 74472-38-1
Molecular Formula: C$_{12}$H$_5$Cl$_5$
Molecular Weight: 326.433
Melting Point (°C): 87 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m$^3$ or mg/L at 25°C):
0.0428 (S$_L$ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00342, 0.00517, 0.00142, 0.00494 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0082 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41 × 10$^{-3}$ (P$_L$ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00599, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)
0.00224 (supercooled liquid P$_L$, GC-RI correlation, Fischer et al. 1992)
log (P$_L$/Pa) = – 4522/(T/K) + 12.50 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
42.56 (calculated-P/C, Burkhard 1984)
31.11 (calculated-QSAR- MCI $\chi$, S abljic & Güsten 1989)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K$_{\text{AW}}$ = – $\Delta H_{\text{f}}$/RT + $\Delta S_{\text{f}}$/R; R is the ideal gas constant, $\Delta H_{\text{f}} = 29 \pm 8$ kJ/mol, $\Delta S_{\text{f}} = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K$_{\text{OW}}$:
6.27 (calculated-TSA, Burkhard 1984)
6.43, 6.40, 6.55, 6.38 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.49 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.44 (recommended, Sangster 1993)
6.4654 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K$_{\text{OA}}$:
9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K$_{\text{B}}$:
Polychlorinated Biphenyls (PCBs)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.07 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI 1, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1 = 9$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.07$ d$^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 11$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.116 2,3,4,5,6-Pentachlorobiphenyl (PCB-116)

Common Name: 2,3,4,5,6-Pentachlorobiphenyl
Synonym: PCB-116, 2,3,4,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5,6-pentachlorobiphenyl
CAS Registry No: 18259-05-7
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
123.5 (Lide 2003)
Boiling Point (°C):
381 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm³ at 20°C): 1.2803
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
21.80 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{ fus} (J/mol K):
54.81 (Miller et al. 1984)
54.83, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.108 (mp at 123.5°C)
0.105 (Mackay et al. 1980; Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0068 (generator column-GC/ECD, Weil et al. 1974)
0.0207 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00548 (generator column-GC/ECD, Miller et al. 1984,1985)
0.00139, 0.00517, 0.00158, 0.00608 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00401 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0136 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000788, 0.000394, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00341 (supercooled liquid P_l, GC-RI correlation, Burkhard et al. 1985b)
0.0024 (supercooled liquid P_l, GC-RI correlation, Fischer et al. 1992)
log (P_l/Pa) = – 4522/(T/K) + 12.53 (GC-RT correlation, Falconer & Bidleman 1994)
0.00326 (P_l, calculated-MCI 3χ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
Henry’s Law Constant (Pa m³/mol at 25°C):
18.34 (calculated-P/C, Burkhard et al. 1985b)
23.41 (calculated-QSPR-MCI χ, Sabljic et al. 1989)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – ΔH_{f}^{H}/RT + ΔS_{f}^{H}/R; R is the ideal gas constant, ΔH_{f} = 29 ± 8 kJ/mol, ΔS_{f} = 0.06 ± 0.01 kJ/mol*K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 6.85 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
- 7.49 (calculated-f const., Yalkowsky et al. 1983)
- 6.30 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 6.30; 6.70, 6.40, 6.65, 6.32 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.754 ± 0.015 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 6.25 (HPLC-k' correlation, Noegrohati & Hammers 1992)
- 5.46 (recommended, Sangster 1993)
- 6.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$
- 9.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:

Bioaccumulation Factor, log $BAF$:
- 5.46 (fish, lipid based-L/kg(Ip), Thomann 1989)

Sorption Partition Coefficient, log $K_{OC}$:
- 5.94 (suspended particulate matter, calculated-$K_{sp}$, Burkhard 1984)
- 4.791 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

- $k_{OH}$(calc) = (0.2–0.4) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{OH}$(calc) = (0.3–0.9) $\times$ 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:
- k$_2$ > 0.0007 d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2}$ > 1000 d in rainbow trout, and $t_{1/2}$ = 100 d in its muscle, 100 d (Niimi & Oliver 1983).
7.1.1.117 2,3,4',5,6-Pentachlorobiphenyl (PCB-117)

Common Name: 2,3,4',5,6-Pentachlorobiphenyl
Synonym: PCB-117, 2,3,4',5,6-pentachloro-1,1'-biphenyl
Chemical Name: 2,3,4',5,6-pentachlorobiphenyl
CAS Registry No: 68194-11-6
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C): 115 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
Entropy of Fusion, ∆S_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0457 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0042, 0.00651, 0.0248, 0.00494 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.23 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00561, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
log (P/mmHg) = 11.10 – 4800/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00257 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
37.29 (calculated-P/C, Burkhard 1984)
25.13 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln KₐW = – ∆H_H/RT + ∆S_H/R; R is the ideal gas constant, ∆H_H = 29 ± 8 kJ/mol, ∆S_H = 0.06 ± 0.01 kJ/mol-K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_ow:
6.25 (calculated-TSA, Burkhard 1984)
6.37, 6.33, 6.49, 6.28 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.39 (recommended, Sangster 1993)
6.4587 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_oa:
9.20 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Polychlorinated Biphenyls (PCBs)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.05 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.118 2,3’,4,4’,5-Pentachlorobiphenyl (PCB-118)

Common Name: 2,3’,4,4’,5-Pentachlorobiphenyl
Synonym: PCB-118, 2,3’,4,4’,5-pentachloro-1,1’-biphenyl
Chemical Name: 2,3’,4,4’,5-pentachlorobiphenyl
CAS Registry No: 31508-00-6
Molecular Formula: C12H5Cl5
Molecular Weight: 326.433

Melting Point (°C):
106 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
109 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³):
289.1  (calculated-Le Bas method at normal boiling point)
224.5  (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔHfus (kJ/mol):

Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.158 (Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.01344  (20°C, supercooled liquid, Murphy et al. 1987)
0.0153  (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.00107; 0.00198 (generator column-GC/ECD; estimated, Hong & Qiao 1995)
0.00207*  (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.

0.0290, 0.0223(supercooled liquid Sₗ; derivation of literature-derived value, final-adjusted value, Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00120  (P₁ supercooled liquid, GC-RT correlation, Bidleman 1984)
9.62 × 10⁻⁴  (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167  (GC-RI correlation, Burkhard et al. 1985b)
0.00123, 0.00104 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54 × 10⁻⁴  (20°C, supercooled liquid P₁, Murphy et al. 1987)
8.32 × 10⁻⁴, 1.12 × 10⁻³ (supercooled liquid P₁; GC-RI correlation, different stationary phases, Fischer et al. 1992)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
40.8 (concn ratio-GC, Murphy et al. 1983)
8.61 (20°C, gas stripping-GC, Murphy et al. 1987)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polychlorinated Biphenyls (PCBs)</td>
<td>11.75 (calculated-QSPR-MCI $\chi$, Sabljic &amp; Güsten 1989)</td>
</tr>
<tr>
<td></td>
<td>12.73 (calculated-QSPR, Dunnivant et al. 1992)</td>
</tr>
<tr>
<td></td>
<td>3.94 (calculated-QSPR, Achman et al. 1993)</td>
</tr>
<tr>
<td></td>
<td>36.12* ± 1.0 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)</td>
</tr>
<tr>
<td></td>
<td>$\ln K_{\text{AW}} = 15.877 - 5989.9/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)</td>
</tr>
<tr>
<td></td>
<td>$K_{\text{AW}} = \exp[-(49.8/kJ\cdot mol^{-1})/R T] + (0.132/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314 \text{ J}\cdot K^{-1}\cdot \text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)</td>
</tr>
<tr>
<td></td>
<td>36.3 (exptl. data, Bamford et al. 2002)</td>
</tr>
<tr>
<td></td>
<td>$\ln K_{\text{AW}} = -\Delta H_g/RT + \Delta S_g/R$; $R$ is the ideal gas constant, $\Delta H_g = 50 \pm 6$ kJ/mol, $\Delta S_g = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002) — see Comment by Goss et al. 2004</td>
</tr>
<tr>
<td></td>
<td>32.36, 14.45 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)</td>
</tr>
<tr>
<td></td>
<td>$\log H/(Pa \cdot m^3/mol) = -2699/(T/K) + 10.56$ (LDV linear regression of literature data, Li et al. 2003)</td>
</tr>
<tr>
<td></td>
<td>$\log H/(Pa \cdot m^3/mol) = -3289/(T/K) + 12.19$ (FAV final adjusted eq., Li et al. 2003)</td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:</td>
<td>7.42 (HPLC-RT correlation, Shaw &amp; Connell 1982)</td>
</tr>
<tr>
<td></td>
<td>6.66, 7.12 (HPLC-κ correlation, Rapaport &amp; Eisenreich 1984)</td>
</tr>
<tr>
<td></td>
<td>6.57 (RP-HPLC-κ correlation, Brodsky &amp; Ballschmitter 1988)</td>
</tr>
<tr>
<td></td>
<td>6.74 (calculated-TSA, Hawker &amp; Connell 1988a)</td>
</tr>
<tr>
<td></td>
<td>6.24 (generator column-GC, Larsen et al. 1992)</td>
</tr>
<tr>
<td></td>
<td>6.57 (recommended, Sangster 1993)</td>
</tr>
<tr>
<td></td>
<td>6.49 (generator column-GC/ECD, Yeh &amp; Hong 2002)</td>
</tr>
<tr>
<td></td>
<td>6.49, 6.69 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)</td>
</tr>
<tr>
<td>Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:</td>
<td>10.08* (20°C, generator column-GC, measured range –10 to 30°C, Harner &amp; Bidleman 1996)</td>
</tr>
<tr>
<td></td>
<td>$\log K_{\text{OA}} = -5.92 + 4693/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner &amp; Bidleman 1996)</td>
</tr>
<tr>
<td></td>
<td>11.13, 10.04; 10.02 (0, 20°C, multi-column GC-κ correlation; calculated at 20°C, Zhang et al. 1999)</td>
</tr>
<tr>
<td></td>
<td>9.86 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)</td>
</tr>
<tr>
<td></td>
<td>9.80, 9.36 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)</td>
</tr>
<tr>
<td></td>
<td>$\log K_{\text{OA}} = 4646/(T/K) - 6.22$ (FAV final adjusted eq., Li et al. 2003)</td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF or log $K_{\text{B}}$:</td>
<td>3.60–5.19 (various marine species, mean dry weight, Hope et al. 1998)</td>
</tr>
<tr>
<td></td>
<td>5.43 (Baltic Sea blue mussels, flow-through exp, dry wt., Gustafsson et al. 1999)</td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log $K_{\text{OC}}$:</td>
<td>6.16 (suspended particulate matter, calculated-$K_{\text{OW}}$, Burkhard 1984)</td>
</tr>
<tr>
<td></td>
<td>4.88 (as log $K_{\text{b}}$, association coefficient with marine humic substance, calculated-$\chi$, Sabljic et al. 1989)</td>
</tr>
<tr>
<td></td>
<td>5.81 (soil from Ispra near Lake Maggiore, Italy, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)</td>
</tr>
<tr>
<td></td>
<td>5.20 (colloids and micro-particulates, GC/ECD, Murray &amp; Andren 1992)</td>
</tr>
<tr>
<td></td>
<td>5.80 (calculated-$K_{\text{b}}$, Girvin &amp; Scott 1997)</td>
</tr>
<tr>
<td></td>
<td>5.52 (soil, calculated-Characteristic Root Index CRI, Saçan &amp; Balcioğlu 1996)</td>
</tr>
<tr>
<td></td>
<td>4.79–7.42 (range, calculated from sequential desorption of 11 urban soils; Krauss &amp; Wilcke 2001)</td>
</tr>
<tr>
<td></td>
<td>5.46; 6.03, 6.67, 6.26 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of exp 1,2,3-solvophobic approach, Krauss &amp; Wilcke 2001)</td>
</tr>
<tr>
<td></td>
<td>6.16–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)</td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log $K_{\text{P}}$ of log $K_{\text{d}}$:</td>
<td>5.55–5.82 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)</td>
</tr>
<tr>
<td></td>
<td>5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray &amp; Andren 1992)</td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{hal}$. 

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 0.034$ d$^{-1}$ with an elimination $t_{\text{hal}} = 20.3$ d (earthworm, Belfroid et al. 1995)

$k_2 = 0.007$ d$^{-1}$ with $t_{\text{hal}} = 103$ d and $k_2 = 0.013$ d$^{-1}$ with $t_{\text{hal}} = 53$ d for food concn of 20 ng/g and 133 ng/g respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 14$ L d$^{-1}$ g$^{-1}$ dry wt.; $k_2 = 0.052$ d$^{-1}$ (Baltic Sea blue mussels, flow-through exp., Gustafsson et al. 1999)

$k_2 = 0.052$ d$^{-1}$ (Baltic Sea blue mussels, flow-through exp., Gustafsson et al. 1999)

$k_1 = 6$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.06$ d$^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004$ d$^{-1}$ with $t_{\text{hal}} = 180$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d$^{-1}$ with $t_{\text{hal}} = 225$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives: $t_{\text{hal}} = 155$ to $>1000$ d for trout, $t_{\text{hal}} = 62–101$ d for trout muscle; $t_{\text{hal}} = 73$ to $>200$ d for carp for pentachlorobiphenyls (Niimi 1987);

elimination $t_{\text{hal}} = 20.3$ d from earthworm (Belfroid et al. 1995)

elimination $t_{\text{hal}} = 95$ d in rainbow trout, based on 228 d of elimination (Coristine et al. 1996)

depuration $t_{\text{hal}} = 53–103$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical half-life to reach 90% steady-state tissue concn 13.3 d (Baltic Sea blue mussels, flow-through exp., Gustafsson et al. 1999);

elimination $t_{\text{hal}} = 12$ d in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{\text{hal}} = 180$ d for high-dose treatment, $t_{\text{hal}} = 225$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
TABLE 7.1.1.18.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3′,4,4′,5-pentachlorobiphenyl (PCB 118) at various temperatures and reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Huang &amp; Hong 2002</td>
<td>Bamford et al. 2000</td>
<td>Harner &amp; Bidleman 1996</td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
</tr>
<tr>
<td>5</td>
<td>5.85 × 10⁻¹</td>
<td>4</td>
</tr>
<tr>
<td>15</td>
<td>1.22 × 10⁻³</td>
<td>11</td>
</tr>
<tr>
<td>25</td>
<td>2.07 × 10⁻³</td>
<td>18</td>
</tr>
<tr>
<td>35</td>
<td>3.31 × 10⁻³</td>
<td>25</td>
</tr>
<tr>
<td>31</td>
<td></td>
<td>31</td>
</tr>
</tbody>
</table>

\[
\ln x = A - \frac{B}{(T/K)}
\]

eq. 1

\[
\ln K_{AW} = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}
\]

\[
\Delta H_{sol}/(kJ \text{ mol}^{-1}) = 89.86
\]

\[
\Delta H/(kJ \cdot \text{mol}^{-1}) = 49.8 \pm 5.8
\]

\[
\Delta S/(J \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) = 132 \pm 18
\]

FIGURE 7.1.1.18.1 Logarithm of mole fraction solubility, Henry’s law constant and K_{OA} versus reciprocal temperature for 2,3′,4,4′,5-pentachlorobiphenyl (PCB-118).
7.1.1.119 2,3',4',4',6-Pentachlorobiphenyl (PCB-119)

Common Name: 2,3',4',4',6-Pentachlorobiphenyl
Synonym: PCB-119, 2,3',4',4',6-pentachloro-1,1'-biphenyl
Chemical Name: 2,3',4',4',6-pentachlorobiphenyl
CAS Registry No: 56558-17-9
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0353 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00326, 0.00375, 0.00411, 0.00529 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.48 × 10⁻³ (Pₗ supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00269, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)
0.00288 (supercooled liquid Pₗ, GC-RI correlation, Fischer et al. 1992)
$\log (Pₗ/P_a) = -4522/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
22.90 (calculated-P/C, Burkhard 1984)
46.10 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
5.97 (calculated-QSPR, Achman et al. 1993)
31.46 (calculated-QSPR, Dunnivant et al. 1992)
31.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
50.0 (from 11°C expnl. data and compensation point, Bamford et al. 2002)
$\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{fus}} = 20 \pm 5$ kJ/mol, $\Delta S_{\text{fus}} = 0.03 \pm 0.02$ kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
6.36 (calculated-TSA, Burkhard 1984)
6.44, 6.49, 6.33, 6.35 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.40 (recommended, Sangster 1993)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.4124 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:
9.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
6.16 (suspended particulate matter, Burkhard 1984)
4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_b$, calculated-MCI 1χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(\text{calc}) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.120 2,3',4,5,5'-Pentachlorobiphenyl (PCB-120)

Common Name: 2,3',4,5,5'-Pentachlorobiphenyl
Synonym: PCB-120, 2,3',4,5,5'-pentachloro-1,1'-biphenyl
Chemical Name: 2,3',4,5,5'-pentachlorobiphenyl
CAS Registry No: 68194-12-7
Molecular Formula: C_{12}H_5Cl_5
Molecular Weight: 326.433

Melting Point (°C):
- 77 (Shiu & Mackay 1986)
- 77, 93 (exptl., estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C): 
Density (g/cm³):
- Molar Volume (cm³/mol):
  - 289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C, F:
- 0.306 (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \), Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0295 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- \( 1.42 \times 10^{-3} \) (P_L supercooled liquid, Burkhard et al. 1985a)
- 0.00735, 0.00155, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
- 0.00197, 0.00203 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 15.71 (calculated-P/C, Burkhard 1984)
- 40.94 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
- 6.57 (wetted wall column-GC/ECD, Brunner et al. 1990)
- 24.87 (calculated-QSPR, Dunnivant et al. 1992)
- 36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[ \ln K_{\text{AW}} = -\Delta H_{\text{g}}/RT + \Delta S_{\text{g}}/R; \ R \text{ is the ideal gas constant, } \Delta H_{\text{g}} = 56 \pm 17 \text{ kJ/mol, } \Delta S_{\text{g}} = 0.15 \pm 0.01 \text{ kJ/mol-K} \]

Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
- 5.22, 5.68 (HPLC-K' correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 6.41 (calculated-TSA, Burkhard 1984)
- 5.68 (quoted, Sangster 1993)
- 6.79 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.772 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

© 2006 by Taylor & Francis Group, LLC
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, \( \log K_{OA} \):
- 9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):

Sorption Partition Coefficient, \( \log K_{OC} \):
- 6.32 (suspended particulate matter, Burkhard 1984)
- 4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient \( \log K_h \), calculated-MCI \( \chi \), Sabljic et al. 1989)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{½} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) as indicated, *data at other temperatures see reference:
- \( k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 60–120 \text{ d} \), due to gas-phase loss process at room temp. (Atkinson 1987)
- \( k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 16–48 \text{ d} \) at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.121 2,3′,4,5′,6-Pentachlorobiphenyl (PCB-121)

- **Chemical Name:** 2,3′,4,5′,6-pentachlorobiphenyl
- **Synonym:** PCB-121, 2,3′,4,5′,6-pentachloro-1,1′-biphenyl
- **CAS Registry No.:** 56558-18-0
- **Molecular Formula:** C_{12}H_{5}Cl_{5}
- **Molecular Weight:** 326.433
- **Melting Point (°C):**
  - 91 (estimated, Abramowitz & Yalkowsky 1990)

**Boiling Point (°C):**

**Density (g/cm³):**

**Molar Volume (cm³/mol):**

289.1 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:**

**Water Solubility (g/m³ or mg/L at 25°C):**

- 0.0311 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.00411 (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**

- 3.68 × 10⁻³ (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 0.00735, 0.00396, 0.000154 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
- 0.00483, 0.00608 (supercooled liquid P_l, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 0.00501 (supercooled liquid P_l: GC-RI correlation, Fischer et al. 1992)

\[
\log (P_l/P_a) = -4522/(T/K) + 12.85 \quad \text{(GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)}
\]

**Henry’s Law Constant (Pa·m³/mol at 25°C):**

- 38.50 (calculated-P/C, Burkhard 1984)
- 75.39 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
- 56.59 (calculated-QSPR, Dunnivant et al. 1992)
- 44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[
\ln K_{aw} = -\Delta H_{f}^{\circ}/RT + \Delta S_{f}^{\circ}/R; \quad R \text{ is the ideal gas constant, } \Delta H_{f} = 29 ± 8 \text{ kJ/mol, } \Delta S_{f} = 0.06 ± 0.01 \text{ kJ/mol·K} \quad \text{(Bamford et al. 2002)—see Comment by Goss et al. 2004)
\]

**Octanol/Water Partition Coefficient, log K_{ow}:**

- 6.39 (calculated-TSA, Burkhard 1984)
- 6.63, 6.60, 6.19, 6.28 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.42 (recommended, Sangster 1993)
- 6.5572 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

**Octanol/Air Partition Coefficient, log K_{oa}:**

8.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_\text{b}$:

Sorption Partition Coefficient, log $K_{\text{OC}}$:
- 6.19 (suspended particulate matter, Burkhard 1984)
- 4.704 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{\text{as}}$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{\text{OH}}(\text{calc}) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
- $k_{\text{OH}}(\text{calc}) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 60–120 d for pentachlorobiphenyls (Atkinson 1987);
- calculated tropospheric lifetime of 16–48 d for pentachlorobiphenyls (Kwok et al. 1995).
7.1.1.122 2,3,3′,4′,5′-Pentachlorobiphenyl (PCB-122)

Common Name: 2,3,3′,4′,5′-Pentachlorobiphenyl
Synonym: PCB-122
Chemical Name: 2,3,3′,4′,5′-pentachlorobiphenyl
CAS Registry No: 76842-07-4
Molecular Formula: C\textsubscript{12}H\textsubscript{5}Cl\textsubscript{5}
Molecular Weight: 326.433
Melting Point (°C): 111 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):

0.0408 (\(S_L\) supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0128 (20°C, supercooled liquid, Murphy et al. 1987)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

7.76 \times 10^{-4} (\(P_L\) supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.000854, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI \(\chi\), Burkhard et al. 1985b)
9.93 \times 10^{-4}, 7.23 \times 10^{-4} (supercooled liquid \(P_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.21 \times 10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
log \((P_L/P_a) = -4688/(T/K) + 12.72\) (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa-m\textsuperscript{3}/mol at 25°C):

6.21 (calculated-P/C, Burkhard 1984)
6.08 (20°C, calculated-P/C, Murphy et al. 1987)
13.88 (calculated-QSPR-MCI \(\chi\), Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R; R is the ideal gas constant, \(\Delta H_{\text{fus}} = 56 \pm 17\) kJ/mol, \(\Delta S_{\text{fus}} = 0.15 \pm 0.01\) kJ/mol-K

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):

6.29 (calculated-TSA, Burkhard 1984)
6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.4986 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):

9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.09 (suspended particulate matter, Burkhard 1984)
- 4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:

- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
  - tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.123 2,3′,4,4′,5′-Pentachlorobiphenyl (PCB-123)

Common Name: 2,3′,4,4′,5′-Pentachlorobiphenyl  
Synonym: PCB-123, 2,3′,4,4′,5′-pentachloro-1,1′-biphenyl  
Chemical Name: 2,3′,4,4′,5′-pentachlorobiphenyl  
CAS Registry No: 65510-44-3  
Molecular Formula: C_{12}H_{5}Cl_{5}  
Molecular Weight: 326.433  
Melting Point (°C):  
125 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
289.1 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:  

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):  
0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
0.000424 (generator column-GC/ECD, Hong & Qiao 1995)  
0.000899 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004.  
0.000299, 0.000512, 0.000899, 0.00155 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)  

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
9.08 × 10⁻⁴ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00099 (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)  
0.0013, 0.00095 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
0.000933 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)  
log (P_L/Pa) = –4688/(T/K) + 12.84 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  

Henry’s Law Constant (Pa·m³/mol at 25°C):  
8.805 (calculated-P/C, Burkhard 1984)  
17.65 (calculated-QSPR, Dunnivant et al. 1992)  
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 56 ± 17 kJ/mol, ΔS_{fus} = 0.15 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004  

Octanol/Water Partition Coefficient, log K_{ow}:  
6.63, 6.60, 6.19, 6.28 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
6.74 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)  
6.64 (recommended, Sangster 1993)  
6.4832 (calculated-molecular properties MNDO-AMI, Makino 1998)  
6.50 (generator column-GC/ECD, Yeh & Hong 2002)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
9.83 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
6.16 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
4.884 (as log $K_a$, association coefficient with marine humic substance, calculated-$\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 15–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation half-life of 21.2 min when irradiated in a TiO$_2$ semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).
Ground water:
Sediment:
Soil:
Biota: reported biological half-lives for pentachlorobiphenyls: $t_{b1} = 155$ to $> 1000$ d for trout, $t_{b2} = 62–101$ d for trout muscle; $t_{b3} = 73$ to $> 200$ d for carp (Niimi 1987)
7.1.1.124 2,3',4',5,5'-Pentachlorobiphenyl (PCB-124)

Common Name: 2,3',4',5,5'-Pentachlorobiphenyl
Synonym: PCB-124, 2',3,4,5,5'-pentachloro-1,1'-biphenyl, 2',3,4,5,5'-pentachlorobiphenyl
Chemical Name: 2,3',4',5,5'-pentachlorobiphenyl
CAS Registry No: 70424-70-3
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C):
99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₜₜ (kJ/mol):
Entropy of Fusion, ΔSₜₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0336 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00158 (20°C, supercooled liquid, Murphy et al. 1987)
0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.01 × 10⁻³ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00112 (GC-RI correlation, Burkhard et al. 1985b)
2.60 × 10⁻⁴ (20°C, supercooled liquid P₁, Murphy et al. 1987)
log (P₁/Pa) = –4688/(T/K) + 12.62 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
9.84 (calculated-P/C, Burkhard 1984)
5.37 (20°C, calculated-P/C, Murphy et al. 1987)
19.76 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.70 (calculated-QSPR, Achman et al. 1993)
17.65 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₘₜₜ = –ΔHᵢₒ/RT + ΔSᵢₒ/R; R is the ideal gas constant, ΔHᵢₒ = 56 ± 17 kJ/mol, ΔSᵢₒ = 0.15 ± 0.01 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₐₒₜ:
6.36 (calculated-TSA, Burkhard 1984)
6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6178 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₐₒₐ:
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log Kₗ:

© 2006 by Taylor & Francis Group, LLC
Sorption Partition Coefficient, log $K_{OC}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.16</td>
<td>(suspended particulate matter, Burkhard 1984)</td>
</tr>
<tr>
<td>4.884</td>
<td>(marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, calculated-MCI $\chi$, Sabljic et al. 1989)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Volatileization:**
**Photolysis:**
**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)

**Hydrolysis:**
**Biodegradation:**
**Biotransformation:**
**Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.125 2,3',4',5',6-Pentachlorobiphenyl (PCB-125)

Common Name: 2,3',4',5',6-Pentachlorobiphenyl
Synonym: PCB-125
Chemical Name: 2,3',4',5',6-pentachlorobiphenyl
CAS Registry No: 74472-39-2
Molecular Formula: C₁₂H₅Cl₅
Molecular Weight: 326.433
Melting Point (°C): 73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH₊ (kJ/mol):
Entropy of Fusion, ΔS₊ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₊ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K₉₅₆:

Octanol/Air Partition Coefficient, log K₉₅₈:

Bioconcentration Factor, log BCF or log K₉₅₈:
Polychlorinated Biphenyls (PCBs)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.09 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{a}$, calculated-MCI 1, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
  - $k_{OH}(calc) = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16–48$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
### PCB-126

**Chemical Name:** 3,3′,4,4′,5-Pentachlorobiphenyl

**Synonym:** PCB-126

**CAS Registry No:** 57465-28-8

**Molecular Formula:** C_{12}H_{5}Cl_{5}

**Molecular Weight:** 326.433

**Melting Point (°C):**
- 106 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

**Boiling Point (°C):**

**Density (g/cm³):**

**Molar Volume (cm³/mol):**
- 289.1 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C, F:**
- 0.158 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**
- 0.0321 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
- 0.000305 (generator column-GC/ECD, Hong & Qiao 1995)
- 0.00133* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
- 2.736 × 10⁻⁴ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 3.05 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
- 4.86 × 10⁻⁴, 2.86 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 3.09 × 10⁻⁴ (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)

**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**
- 2.776 (calculated-P/C, Burkhard et al. 1985)
- 5.471 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
- 8.39 (calculated-QSAR, Dunnivant et al. 1992)
- 21.02* ± 0.83 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
- ln K_{AW} = 35.001 – 11847.5/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
- K_{AW} = exp[-(98.5/kJ·mol⁻¹)/RT] + (0.291/kJ·mol⁻¹·K⁻¹)/R]; where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
- ln K_{AW} = –ΔH_{f} / RT + ΔS_{f} / R; R is the ideal gas constant, ΔH_{f} = 99 ± 9 kJ/mol, ΔS_{f} = 0.29 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
- 21.3 (expnl. data, Bamford et al. 2002)

**Octanol/Water Partition Coefficient, log K_{ow}:**
- 6.38 (calculated-TSA, Burkhard 1984)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- \( 10.61^* \) (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
- \( \log K_{OA} = -5.98 + 4870/(T/K) \); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
- \( 11.77, 10.66; 10.61 (0, 20°C, GC-k' correlation; calculated at 20°C, Zhang et al. 1999) \)
- \( 10.56 \) (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):
- \( 5.81, 7.35 \) (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor BSAF:
- 43 (trout, Niimi 1996)

Sorption Partition Coefficient, \( \log K_{OC} \):
- \( 6.18 \) (suspended particulate matter, calculated-\( K_{OW} \), Burkhard 1984)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

- Volatilization:
- Oxidation:
  - rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO\(_3\) radical and \( k_{O_3} \) with O\(_3\) as indicated, *data at other temperatures see reference:
  - \( k_{OH}(calc) = (0.2–0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 60–120 \text{ d, due to gas-phase loss process at room temp.} \) (Atkinson 1987)
  - \( k_{OH}(calc) = (0.3–0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for pentachlorobiphenyls, and the tropospheric lifetime \( \tau(calc) = 16–48 \text{ d at room temp.} \) (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:

- Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
  - \( k_1 = 5 \) (food lipid mg)/(g worm lipid-d); \( k_2 = 0.05 \text{ d}^{-1} \) (earthworm, Wågman et al. 2001)
  - \( k_2 = 0.0137 \text{ d}^{-1} \) with \( t_{1/2} = 51 \text{ d} \) (newly contaminated oysters, Gardinalli et al. 2004)
  - \( k_2 = 0.0116 \text{ d}^{-1} \) with \( t_{1/2} = 60 \text{ d} \) (chronically contaminated oysters, Gardinalli et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

- Surface water: photodegradation \( t_{1/2} = 304 \text{ min} \) when irradiated in a TiO\(_2\) semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

- Ground water:

- Soil:

- Biota: reported biological half-lives for pentachlorobiphenyls: \( t_{1/2} = 155 \text{ to } 1000 \text{ d} \) for trout, \( t_{1/2} = 62–101 \text{ d} \) for trout muscle; \( t_{1/2} = 73 \text{ to } 200 \text{ d} \) for carp (Niimi 1987);
- elimination \( t_{1/2} = 13 \text{ d} \) in earthworm given contaminated food (Wågman et al. 2001)
- Depuration \( t_{1/2} = 51 \text{ d} \) for newly contaminated oysters, and \( t_{1/2} = 60 \text{ d} \) for chronically contaminated oysters (Gardinalli et al. 2004)
### TABLE 7.1.1.126.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3′,4,4′,5-pentachlorobiphenyl (PCB 126) at various temperatures and reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Huang &amp; Hong 2002</strong></td>
<td><strong>Bamford et al. 2000</strong></td>
<td><strong>Harner &amp; Bidleman 1996</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>$6.30 \times 10^{-4}$</td>
<td>4</td>
</tr>
<tr>
<td>15</td>
<td>$9.64 \times 10^{-4}$</td>
<td>11</td>
</tr>
<tr>
<td>25</td>
<td>$1.33 \times 10^{-3}$</td>
<td>18</td>
</tr>
<tr>
<td>35</td>
<td>$1.60 \times 10^{-3}$</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>31</td>
</tr>
</tbody>
</table>

$\ln x = A - B/(T/K)$

$\ln K_{AW} = -\Delta H/RT + \Delta S/R$

$A = 35.012$

$B = \Delta H/R$

$\Delta H/(kJ mol^{-1}) = 93.25$

$\Delta S/(J·mol^{-1}·K^{-1}) = 291 \pm 32$

**mp/°C**: 160–161

$\Delta H_{sol}/(kJ mol^{-1}) = 22.3$

$\Delta H/(kJ·mol^{-1}) = 98.5 \pm 9.4$

$\Delta S/(J·mol^{-1}·K^{-1}) = 22.3$

**FIGURE 7.1.1.126.1** Logarithm of mole fraction solubility, Henry's law constant and $K_{OA}$ versus reciprocal temperature for 3,3′,4,4′,5-pentachlorobiphenyl (PCB-126).
7.1.1.127 3,3′,4,5,5′-Pentachlorobiphenyl (PCB-127)

Common Name: 3,3′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-127
Chemical Name: 3,3′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 39635-33-1
Molecular Formula: C_{12}H_{5}Cl_{5}
Molecular Weight: 326.433
Melting Point (°C):
135 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0285 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.000651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.04 × 10⁻⁴ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000449 (GC-RI correlation, Burkhard et al. 1985b)
7.80 × 10⁻⁴, 5.38 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
\[ \log (P₁/Pa) = -4956/(T/K) + 13.51 \] (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
4.64 (calculated-P/C, Burkhard 1984)
34.45 (calculated-QSAR-MCI \( \chi \), Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
21.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\[ \ln K_{\text{AW}} = -\Delta H/RT + \Delta S/R; \] R is the ideal gas constant, \( \Delta H = 99 \pm 9 \) kJ/mol, \( \Delta S = 0.29 \pm 0.03 \) kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
6.42 (calculated-TSA, Burkhard 1984)
6.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.8023 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
10.53 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log \( K_{\text{B}} \):
Sorption Partition Coefficient, log \( K_{\text{OC}} \):
6.22 (suspended particulate matter, Burkhard 1984)
Environmental Fate Rate Constants, k, and Half-Lives, $\tau$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$\tau_{(calc)} = (0.2–0.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau_{(calc)} = 60–120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$\tau_{(calc)} = (0.3–0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau_{(calc)} = 16–48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.128 2,2',3,3',4,4'-Hexachlorobiphenyl (PCB-128)

![Chemical structure of 2,2',3,3',4,4'-Hexachlorobiphenyl](image)

Common Name: 2,2',3,3',4,4'-Hexachlorobiphenyl
Synonym: PCB-128, 2,2',3,3',4,4'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',4,4'-hexachlorobiphenyl
CAS Registry No: 38380-07-3
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
151 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.3482
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.83 (Miller et al. 1984)
29.20 (Ruelle et al. 1993; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
68.62 (Miller et al. 1984; Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0582 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
4.40 × 10⁻⁴ (generator column-GC/ECD, Weil et al. 1974)
9.90 × 10⁻⁴ (shake flask-GC/ECD, Dexter & Pavlou 1978)
2.85 × 10⁻⁴ (generator column-GC/ECD, Miller et al. 1984,1985)
0.0067 (20°C, supercooled liquid Sₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
2.74 × 10⁻³, 2.17 × 10⁻², 9.07 × 10⁻², 1.54 × 10⁻¹ (RP-HPLC-k’ correlation, different stationary and mobile phase, Brodsky & Ballaschmutter 1988)
0.0023 (generator column-GC, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41 × 10⁻⁴ (supercooled liquid Pₜ, GC-RT correlation, Bidleman 1984)
3.59 × 10⁻⁴ (supercooled liquid Pₜ, Burkhard 1984)
2.31 × 10⁻⁵ (GC-RI correlation, Burkhard et al. 1985a)
3.59 × 10⁻⁴ (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al. 1985b)
3.67 × 10⁻⁴, 2.94 × 10⁻⁴ (supercooled liquid Pₜ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.83 × 10⁻⁵ (20°C, supercooled liquid Pₜ, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
3.67 × 10⁻⁴, 2.94 × 10⁻⁴, 3.41 × 10⁻⁴ (supercooled liquid Pₜ, GC-RT correlation, Foreman & Bidleman 1985)
log (P/Pa) = 11.40 – 5020/(T/K) (GC-RT correlation, Tateya et al. 1988)
1.78 × 10⁻³, 3.31 × 10⁻³ (supercooled liquid Pₜ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P/Pa) = -4881/(T/K) + 12.91 (GC-RT correlation, Falconer & Bidleman 1994)
(2.90 – 154.0) × 10⁻⁷; (9.80 – 35.9) × 10⁻⁸ (literature solid Pₜ range; supercooled liquid Pₜ range, Delle Site 1997)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
50.66 (calculated, Murphy et al. 1983)
6.85 (calculated-P/C, Burkhard et al. 1985b)
11.91 (calculated-P/C, Shiu & Mackay 1986)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octanol/Water Partition Coeff.</td>
<td>log $K_{OW}$</td>
</tr>
<tr>
<td></td>
<td>7.44 (RP-TLC-RT correlation, Bruggeman et al. 1982)</td>
</tr>
<tr>
<td></td>
<td>6.98 (generator column-GC/ECD, Miller et al. 1984, 1985)</td>
</tr>
<tr>
<td></td>
<td>6.14 (HPLC-RT correlation, Rapaport &amp; Eisenreich 1984)</td>
</tr>
<tr>
<td></td>
<td>6.28 (HPLC-RP/MS correlation, Burkhard et al. 1985c)</td>
</tr>
<tr>
<td></td>
<td>6.50, 6.67, 6.83, 6.73 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky &amp; Ballschmier 1988)</td>
</tr>
<tr>
<td></td>
<td>6.98 (generator column-GC/ECD, Doucette &amp; Andren 1988)</td>
</tr>
<tr>
<td></td>
<td>7.24 (calculated-UNIFAC activity coefficients, Banerjee &amp; Howard 1988)</td>
</tr>
<tr>
<td></td>
<td>7.321 $\pm$ 0.027 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn &amp; Hermens 1990)</td>
</tr>
<tr>
<td></td>
<td>6.98, 6.87; 6.92, 6.87 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)</td>
</tr>
<tr>
<td></td>
<td>6.71 (HPLC-k’ correlation, Neogrohati &amp; Hammers 1992)</td>
</tr>
<tr>
<td></td>
<td>6.62 (generator column-GC, Larsen et al. 1992)</td>
</tr>
<tr>
<td></td>
<td>6.96 (recommended, Sangster 1993)</td>
</tr>
<tr>
<td></td>
<td>7.32 (recommended, Hansch et al. 1995)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{OA}$:

- 9.93 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 1.0 (poultry, Garten & Trabalka 1983)
- 4.28 (worms, Oliver 1987c)
- 5.77; 7.30 (22°C, zebrafish: log BCF$_w$ wet wt basis; log BCF$_l$ lipid wt basis, Fox et al. 1994)
- 3.20–5.12 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.90–6.03 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 5.77, 7.31 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.41, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:

- 5.05 (calculated-MCI, Koch 1983)
- 6.42 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.06 (calculated-MCI, Bahnick & Doucette 1988)
- 5.26 (marine humic substance, calculated-MCI $\chi$, reported as log $K_{h}$ at 5 mg/L DOC, Sabljic et al. 1989)
- 6.28, 6.17, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 6.0 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.05 (soil, calculated-MCI, Sabljic et al. 1995)
- 5.93 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
- 6.50 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
- 6.00; 5.10 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
Sorption Partition Coefficient, $\log K_{OM}$:
5.05, 5.09 (quoted, calculated-MCI $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\text{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
Photooxidation: calculated room temp. rate constant for hexachlorobiphenyls is $(0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with OH radicals, the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1996).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 4970 \text{ d}^{-1}$; $k_2 = 0.00843 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.009 \text{ d}^{-1}$ with $t_\text{½} = 75 \text{ d}$ and $k_2 = 0.012 \text{ d}^{-1}$ with $t_\text{½} = 59 \text{ d}$ for food concn of 8 ng/g and 99 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005 \text{ d}^{-1}$ with $t_\text{½} = 146 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003 \text{ d}^{-1}$ with $t_\text{½} = 205 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_\text{½} > 1000 \text{ d}$ in rainbow trout, and $t_\text{½} = 89 \text{ d}$ in its muscle (Niimi & Oliver 1983).
Depuration $t_\text{½} = 59–75 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
Depuration $t_\text{½} = 146 \text{ d}$ for high-dose treatment, $t_\text{½} = 205 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.129 2,2',3,3',4,5-Hexachlorobiphenyl (PCB-129)

Common Name: 2,2',3,3',4,5-Hexachlorobiphenyl
Synonym: PCB-129, 2,2',3,3',4,5-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',4,5-hexachlorobiphenyl
CAS Registry No: 55215-18-4
Molecular Formula: C\textsubscript{12}H\textsubscript{4}Cl\textsubscript{6}
Molecular Weight: 360.878
Melting Point (°C):
85 (Mackay et al. 1980; Bruggeman et al. 1982; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm\textsuperscript{3} at 20°C): 1.3482
Molar Volume (cm\textsuperscript{3}/mol):
310.0 (calculated-Le Bas method at normal boiling point.)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ∆H\textsubscript{fus} (kJ/mol):
Entropy of Fusion, ∆S\textsubscript{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S\textsubscript{fus} = 56 J/mol K), F:
0.256 (Shiu & Mackay 1986)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
0.00085 (generator column-GC/ECD, Weil et al. 1974)
0.0117 (20°C, supercooled liquid S, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00150, 0.00198, 0.000688, 0.00169 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00582 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.76 × 10\textsuperscript{-4} (GC-RI correlation, Burkhard et al. 1985a)
0.00208 (supercooled liquid P\textsubscript{l}, GC-RI correlation, Burkhard et al. 1985b)
4.68 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{l}, GC-RI correlation, Fischer et al. 1992)
log (P\textsubscript{l}/Pa) = – 4816/(T/K) + 12.80 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):
39.52 (calculated-P/C, Burkhard et al. 1985b)
8.61 (calculated-MCI χ, Sabljic & Güsten 1989)
2.94 (wetted-wall column-GC, Brunner et al. 1990)
14.18 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K\textsubscript{AW} = –ΔH\textsubscript{f}/RT + ΔS\textsubscript{f}/R; R is the ideal gas constant, ΔH\textsubscript{f} = 79 ± 18 kJ/mol, ΔS\textsubscript{f} = 0.23 ± 0.06 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K\textsubscript{OW}:
6.50 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.71, 6.71, 6.90, 6.71 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
6.94, 6.70; 6.81, 6.83 (multi-column HPLC-k correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 6.76 (recommended, Sangster 1993)
- 7.32 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.42 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.259 (marine humic substance, calculated-MCI $\chi$, reported as association coefficient log $K_a$ at 5 mg/L DOC, Sabljić 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}$(calc) = $(0.16 \pm 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 29–60 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 156$ d for high-dose treatment, $t_{1/2} = 166$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.130 2,2’,3,3’,4,5’-Hexachlorobiphenyl (PCB-130)

Common Name: 2,2’,3,3’,4,5’-Hexachlorobiphenyl
Synonym: PCB-130, 2,2’,3,3’,4,5’-hexachloro-1,1’-biphenyl
Chemical Name: 2,2’,3,3’,4,5’-hexachloro-1,1’-biphenyl
CAS Registry No: 52663-66-8
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C): 96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0168 (Sₜ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00569 (20°C, supercooled liquid, Murphy et al. 1987)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.35 × 10⁻⁴ (Pₜ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.92 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
1.61 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
4.17 × 10⁻⁴, 5.75 × 10⁻⁴ (supercooled liquid Pₜ; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₜ/Pa) = –4816/(T/K) + 12.89 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
10.84 (20°C, calculated-P/C, Murphy et al. 1987)
19.45 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
3.75 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.44 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{\text{AW}}$ = –$\Delta H_{\text{fus}}$/RT + $\Delta S_{\text{fus}}$/R; R is the ideal gas constant, $\Delta H_{\text{fus}}$ = 79 ± 18 kJ/mol, $\Delta S_{\text{fus}}$ = 0.23 ± 0.06 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
6.98, 7.15; 6.79, 6.78 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.12 (recommended, Sangster 1993)
7.39 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:
9.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.47 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_1/2$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 184$ d for high-dose treatment, $t_{1/2} = 153$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.131 2,2',3,3',4,6-Hexachlorobiphenyl (PCB-131)

Common Name: 2,2',3,3',4,6-Hexachlorobiphenyl  
Synonym: PCB-131, 2,2',3,3',4,6-hexachloro-1,1'-biphenyl  
Chemical Name: 2,2',3,3',4,6-hexachlorobiphenyl  
CAS Registry No: 61798-70-7  
Molecular Formula: C\textsubscript{12}H\textsubscript{4}Cl\textsubscript{6}  
Molecular Weight: 360.878  
Melting Point (°C):  
\[122\] (estimated, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm\textsuperscript{3}):  
Molar Volume (cm\textsuperscript{3}/mol):  
\[310.0\] (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), $F$:  
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):  
\[0.0151\] (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
\[0.0121\] (20°C, supercooled liquid, Murphy et al. 1987)  
\[0.00120\] (RP-HPLC-k' correlation, Brodsky & Ballischminter 1988)  
\[0.00287\] (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
\[2.62 \times 10^{-3}\] (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
\[0.00285\] (GC-RI correlation, Burkhard et al. 1985b)  
\[0.00126, 0.0107\] (supercooled liquid P\textsubscript{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
\[2.63 \times 10^{-4}\] (20°C, supercooled liquid, Murphy et al. 1987)  
\[6.92 \times 10^{-4}\] (supercooled liquid P\textsubscript{L}, GC-RI correlation, Fischer et al. 1992)  
\[\log (P_{L}/P_{a}) = -4681/(T/K) + 12.80\] (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C or as indicated):  
\[62.82\] (calculated-P/C, Burkhard 1984)  
\[6.59\] (20°C, calculated-P/C, Murphy et al. 1987)  
\[26.24\] (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)  
\[3.95\] (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)  
\[24.53\] (calculated-QSPR, Dunnivant et al. 1992)  
\[68.8\] (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\[\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R\]  
R is the ideal gas constant, $\Delta H_{\text{fus}} = 47 \pm 8$ kJ/mol, $\Delta S_{\text{fus}} = 0.13 \pm 0.03$ kJ/mol·K  
(bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:  
\[6.78\] (RP-HPLC-k' correlation, Brodsky & Ballischminter 1988)  
\[6.97, 6.38; 6.41, 6.44\] (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)  
\[6.78\] (recommended, Sangster 1993)  
\[6.82\] (recommended, Hansch et al. 1995)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 10.92, 9.83 (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
- 10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.51 (suspended particulate matter, Burkhard 1984)
- 5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{0.5}$:
Volatilization:
- Oxidation: rate constant $k$ for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.132 2,2′,3,3′,4,6′-Hexachlorobiphenyl (PCB-132)

![Chemical Structure](image)

Common Name: 2,2′,3,3′,4,6′-Hexachlorobiphenyl
Synonym: PCB-132, 2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6′-hexachlorobiphenyl
CAS Registry No: 38380-05-1
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878

Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
310.0 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):

Entropy of Fusion, ∆S_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0149 (Sₐ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00808 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.155 × 10⁻³ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.27 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
7.58 × 10⁻⁴, 9.08 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62 × 10⁻⁴, 1.0 × 10⁻³ (supercooled liquid P₁; GC-RI correlations, different stationary phase, Fischer et al. 1992)
log (P₁/Pa) = −4681/(T/K) + 12.5, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
27.97 (calculated-P/C, Burkhard 1984)
16.31 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
4.46 (wetted wall column-GC/ECD, Brunner et al. 1990)
2.42 (calculated-QSPR, Achman et al. 1993)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
16.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
59.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\ln K_{AW} = −\Delta H_{fus}/RT + \Delta S_{fus}/R, \ R \ is \ the \ ideal \ gas \ constant, \ \Delta H_{fus} = 61 ± 7 \ kJ/mol, \ \Delta S_{fus} = 0.17 ± 0.02 \ kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
6.70 (HPLC-RT correlation, Shaw & Connell 1982)
6.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.09, 6.77; 6.63, 6.58 (multi-column-HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.20 (recommended, Sangster 1993)
7.04 (recommended, Hansch et al. 1995)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:
11.16, 10.07; 9.96 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{\text{B}}$:

Sorption Partition Coefficient, log $K_{\text{OC}}$:
- 6.52 (suspended particulate matter, Burkhard 1984)
- 5.10 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_{\text{h}}$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatile:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{\text{OH}}(\text{calc}) = (0.16 – 0.5) \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60 \ \text{d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_1 = 0.005 \ \text{d}^{-1}$ with $t_\frac{1}{2} = 136 \ \text{d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.005 \ \text{d}^{-1}$ with $t_\frac{1}{2} = 147 \ \text{d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
  - Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
  - Surface water:
  - Ground water:
  - Sediment:
  - Soil:
    - Biota: depuration $t_\frac{1}{2} = 136 \ \text{d}$ for high-dose treatment, $t_\frac{1}{2} = 147 \ \text{d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.133 2,2′,3,3′,5,5′-Hexachlorobiphenyl (PCB-133)

Common Name: 2,2′,3,3′,5,5′-Hexachlorobiphenyl
Synonym: PCB-133, 2,2′,3,3′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′-hexachlorobiphenyl
CAS Registry No: 35694-04-3
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C): 129 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.0149 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
4.37 × 10⁻⁴ (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.98 × 10⁻⁴ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
8.24 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985b)
8.43 × 10⁻⁴, 0.00110 (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P₁/Pa) = –4816/(T/K) + 13.08 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
19.25 (calculated-P/C, Burkhard 1984)
33.84 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.64 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 79 ± 18 kJ/mol, ΔS_{f} = 0.23 ± 0.06 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
6.72 (calculated-TSA, Burkhard 1984)
6.86 (calculated-TSA, Hawker & Connell 1988a)
6.97, 7.02; 6.66, 6.60 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.63, 7.00 (quoted average values of GC-RV and HPLC-k’ correlations of Risby et al. 1990, Sangster 1993)
7.07 (recommended, Hansch et al. 1995)
6.7470 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.52 (suspended particulate matter, Burkhard 1984)
- 5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.134 2,2′,3,3′,5,6-Hexachlorobiphenyl (PCB-134)

Common Name: 2,2′,3,3′,5,6-Hexachlorobiphenyl
Synonym: PCB-134, 2,2′,3,3′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6-hexachlorobiphenyl
CAS Registry No: 52704-70-8
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878

Melting Point (°C):
- 100 (Mackay et al. 1980; Burkhard et al. 1985a; Kühne et al. 1995; Ruelle & Kesselring 1997)
- 132 (Ran et al. 2002)

Boiling Point (°C): 132 (Ran et al. 2002)

Density (g/cm^3 at 20°C): 1.3482

Molar Volume (cm^3/mol):
- 310.0 (calculated-Le Bas method at normal boiling point)
- 237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
- 0.181 (Mackay et al. 1980; Shiou & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
- 0.00091 (generator column-GC/ECD, Weil et al. 1973)
- 0.0081 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 1.46 \times 10^{-4} (calculated-S \times HLC, Burkhard et al. 1985a)
- 4.83 \times 10^{-4} (GC-RJ correlation, Burkhard et al. 1985a)
- 3.60 \times 10^{-4} (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- \log(P/mmHg) = 11.30 - 4940/(T/K) (GC-RJ correlation, Tateya et al. 1988)
- \log(P_{L}/P_{a}) = -4681/(T/K) + 12.79 (supercooled liquid \( P_{L} \), GC-RJ correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
- 57.76 (Murphy et al. 1983)
- 20.67 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
- 68.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_{H}/RT + \Delta S_{H}/R; \ R \text{ is the ideal gas constant, } \Delta H_{H} = 46 \pm 6 \text{ kJ/mol, } \Delta S_{H} = 0.13 \pm 0.02 \text{ kJ/mol-K} \]

(Bamford et al. 2002)——see Comment by Goss et al. 2004
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 6.81 (generator column-GC/ECD, Doucette & Andren 1987)
- 6.20 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
- 6.22, 6.43; 6.40, 6.44 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.20 (recommended, Sangster 1993)
- 6.91 (recommended, Hansch et al. 1993)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 10.80, 9.71 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
- 9.72 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.49 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.18, 5.16, 5.15, 4.41 (humic substances, in concentrations of 5, 10, 20, 40 mg C/L, reported as log $K_{H}$, Lara & Ernst 1989)
- 5.18, 5.10 (marine humic substances, quoted, calculated-MCI $\chi$, reported as log $K_{H}$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  
  $k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)

- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, and Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
### 7.1.1.135 2,2',3,3',5,6'-Hexachlorobiphenyl (PCB-135)

![Chemical Structure](image)

**Common Name:** 2,2',3,3',5,6'-Hexachlorobiphenyl  
**Synonym:** PCB-135, 2,2',3,3',5,6'-hexachloro-1,1'-biphenyl  
**Chemical Name:** 2,2',3,3',5,6'-hexachlorobiphenyl  
**CAS Registry No:** 52744-13-5  
**Molecular Formula:** C_{12}H_{4}Cl_{6}  
**Molecular Weight:** 360.878  
**Melting Point (°C):** 102  
**Boiling Point (°C):**  
**Density (g/cm³):** 310.0  
**Molar Volume (cm³/mol):**  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**  
**Entropy of Fusion, ΔS_{fus} (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:**  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
- 0.0133 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
- 0.01294 (20°C, supercooled liquid, Murphy et al. 1987)  
- 0.00546 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)  
- 0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
- 1.73 × 10^{-3} (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
- 0.00188 (GC-RI correlation, Burkhard et al. 1985b)  
- 0.00115, 0.00184 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
- 5.07 × 10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)  
- 0.000741, 0.00132 (supercooled liquid P_{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)  
- \log (P_{L}/Pa) = –4861/(T/K) + 12.76 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):**  
- 46.81 (calculated-P/C, Burkhard 1984)  
- 14.19 (20°C, calculated-P/C, Murphy et al. 1987)  
- 30.8 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)  
- 5.67 (wetted wall column-GC/ECD, Brunner et al. 1990)  
- 27.21 (calculated-QSPR, Dunnivant et al. 1992)  
- 26.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
- 69.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
- \ln K_{AW} = –\Delta H_{fus}/RT + \Delta S_{fus}/R; R is the ideal gas constant, \Delta H_{fus} = 45 ± 3 kJ/mol, \Delta S_{fus} = 0.12 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
- 5.94, 7.15 (RP-HPLC-k' correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)  
- 6.32 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)  
- 6.97, 6.95; 6.41, 6.40 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)  
  
© 2006 by Taylor & Francis Group, LLC
Polychlorinated Biphenyls (PCBs)

6.32 (recommended, Sangster 1993)
7.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
10.78, 9.69 (0, 20°C, multicolumn GC-k’ correlation, Zhang et al. 1999)
9.71 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
6.57 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-
molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$
with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$ for hexachlorobiphenyls, and the tropospheric
lifetime $\tau(calc) = 29–60 \text{ d at room temp.}$ (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
$k_1 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 159 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration}
\text{expt.- high-dose treatment, Buckman et al. 2004)}$
$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 192 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration}
\text{expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)}$

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH
radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 159 \text{ d for high-dose treatment, } t_{1/2} = 192 \text{ d for high-dose + enzyme CYPIA-inducing}
\text{compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)}$
7.1.1.136 2,2′,3,3′,6,6′-Hexachlorobiphenyl (PCB-136)

Common Name: 2,2′,3,3′,6,6′-Hexachlorobiphenyl
Synonym: PCB-136, 2,2′,3,3′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,6,6′-hexachlorobiphenyl
CAS Registry No: 38411-22-2
Molecular Formula: C\textsubscript{12}H\textsubscript{4}Cl\textsubscript{6}
Molecular Weight: 360.878
Melting Point (°C):
112.05 (differential scanning calorimetry, Miller et al. 1984)
114.2 (Lide 2003)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):
21.21 (differential scanning calorimetry, Miller et al. 1984)
21.10 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K):
54.81 (Miller et al. 1984)
Fugacity Ratio at 25°C, F:
0.138 (calculated, assuming ΔS\textsubscript{fus} = 56 J/mol K, Shiu & Mackay 1986)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00099 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00603 (generator column-GC/ECD, Miller et al. 1984)
0.00451* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
1.10 × 10\textsuperscript{-3}, 3.25 × 10\textsuperscript{-3}, 4.51 × 10\textsuperscript{-3}, 6.68 × 10\textsuperscript{-3} (4, 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)
ln x = –5484.72/(T/K) – 3.8682; temp range 4–32°C, ΔH\textsubscript{s} = 45.6 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = –2378/(T/K) – 1.679, ΔH\textsubscript{s} = 45.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 2.39 × 10\textsuperscript{-9} exp(0.065·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.0202 (20°C, supercooled liquid S\textsubscript{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
ln x = –3.880235 – 5471.2/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.000531 (GC-RI correlation, Burkhard et al. 1985a)
0.00374 (supercooled liquid P\textsubscript{L}, GC-RI correlation, Burkhard et al. 1985b)
0.00156, 0.00292 (supercooled liquid P\textsubscript{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00127 (20°C, supercooled liquid P\textsubscript{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00158, 0.00331 (supercooled liquid P\textsubscript{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P\textsubscript{L}/Pa) = – 4303/(T/K) + 11.63 (supercooled liquid P\textsubscript{L}, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):

93.22  (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
22.79  (20°C, calculated-P/C, Murphy et al. 1987)
25.54  (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.92   (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.64  (calculated-QSPR, Dunnivant et al. 1992)
45.4   (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
81.5   (from 11°C exptl. data and compensation point, Bamford et al. 2002)—see Comment by Goss et al. 2004

ln K_{AW} = –ΔH_f/RT + ΔS_f/R; R is the ideal gas constant, ΔH_f = 27 ± 5 kJ/mol, ΔS_f = 0.06 ± 0.02 kJ/mol·K
(Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

8.35   (Hansch & Leo 1979)
6.81   (generator column-HPLC, Woodburn et al. 1984)
6.63   (generator column-GC/ECD, Miller et al. 1984)
4.91   (RP-HPLC-RT correlation, Rapoport & Eisenreich 1984)
5.48   (HPLC-RT correlation, Burkhard et al. 1985c)
6.81   (generator column-GC/ECD, Doucette & Andren 1987, 1988)
5.76   (generator column-GC/ECD, Hawker & Connell 1988a)
7.118 ± 0.034 (shake flask/slow stirring-GC, De Brujin et al. 1989; De Bruijn & Hermens)
7.18   (calculated-π const., De Bruijn et al. 1989)
6.63, 6.30; 6.30, 6.24 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.50   (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
6.54   (recommended, Sangster 1993)
7.12   (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.59, 9.53; 9.58 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
9.51   (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

0.86   (poultry, Garten & Trabalka 1983)
5.43; 6.96 (22°C, zebrafish: log BCF_{W} wet wt basis; log BCF_{L} lipid wt basis, Fox et al. 1994)
5.43, 6.96 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.53   (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.53   (suspended solids, 0.7 mg/L, 43.2% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.68   (suspended solids, 6.5 mg/L, 14.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.95, 5.05, 4.95, 4.27 (marine humic substances in concentrations of 5, 10, 20, 40 mg L of DOC, reported as association coefficient log K_{a}, Lara & Ernst 1989)
4.952, 4.942 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_{a}. Observed; calculated-MCI χ, Sabljic et al. 1989)
6.01, 6.06, 5.90 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.04 (5.73–6.35) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{SO3} with NO_{3} radical and k_{O3} with O_{3} or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: 18% at 24 h and 33% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism Alcaligenes eutrophus H850 (Bedard et al. 1986).

Biotransformation:
Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:
\[ k_1 = 4390 \, \text{d}^{-1} ; \quad k_2 = 0.0181 \, \text{d}^{-1} \] (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

\[ k_2 = 0.005 \, \text{d}^{-1} \] with \( t_{1/2} = 132 \, \text{d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

\[ k_2 = 0.005 \, \text{d}^{-1} \] with \( t_{1/2} = 144 \, \text{d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation \( t_{1/2} = 15.0 \, \text{min} \) when irradiated in a TiO₂ semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:
Sediment:
Soil:
Biota: depuration \( t_{1/2} = 132 \, \text{d} \) for high-dose treatment, \( t_{1/2} = 144 \, \text{d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.137 2,2′,3,4,4′,5-Hexachlorobiphenyl (PCB-137)

Common Name: 2,2′,3,4,4′,5-Hexachlorobiphenyl
Synonym: PCB-137, 2,2′,3,4,4′,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5-hexachlorobiphenyl
CAS Registry No: 35694-06-5
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C): 78.0 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘᵤₙ (kJ/mol):
Entropy of Fusion, ΔSₘᵤₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘᵤₙ = 56 J/mol K), F: 0.302 (mp at 78°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0158 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0084 (20°C, supercooled liquid, Murphy et al. 1987)
9.94 × 10⁻⁴, 1.12 × 10⁻³, 7.54 × 10⁻⁴, 1.69 × 10⁻³ (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmied 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.71 × 10⁻³ (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.41 × 10⁻³ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.83 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
1.50 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
3.80 × 10⁻⁴, 3.02 × 10⁻⁴ (supercooled liquid Pₗ; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₗ/Pₐ) = –4816/(T/K) + 12.61 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
55.02 (calculated-P/C, Burkhard 1984)
6.89 (20°C, calculated-P/C, Murphy et al. 1987)
21.08 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
18.82 (calculated-QSPR, Dunnivant et al. 1992)
3.13 (calculated-QSPR, Achman et al. 1993)
13.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
55.0 (from 11°C expvl. data and compensation point, Bamford et al. 2002)
ln Kₐₘₖ = –ΔHₑ/RT + ΔSₑ/R; R is the ideal gas constant, ΔHₑ = 69 ± 8 kJ/mol, ΔSₑ = 0.20 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₐₘₖ:
> 6.89, > 7.71 (RP-HPLC-k’ correlation; uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
7.46 (HPLC-RT correlation, De Kock & Lord 1987)
6.84, 6.87, 6.88, 6.71 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.97, 7.06; 6.82, 6.78 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 9.89 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{B}$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_{a}$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.94 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}(\text{calc}) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 191$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 186$ d for high-dose treatment, $t_{1/2} = 191$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.138 2,2′,3,4,4′,5′-Hexachlorobiphenyl (PCB-138)

Common Name: 2,2′,3,4,4′,5′-Hexachlorobiphenyl
Synonym: PCB-138, 2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′-hexachlorobiphenyl
CAS Registry No: 35065-28-2
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
- 79 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
- 80.5 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C): Density (g/cm³):
Molar Volume (cm³/mol):
- 310.0 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
- 247.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol): Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
- 56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
- 0.286 (calculated, assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K, Mackay et al. 1992)
- 0.285 (calculated-\( \Delta S_{\text{fus}} \) and mp, Passivirta et al. 1995)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
- 0.0159 (supercooled liquid \( S_L \), calculated-TSA, Burkhard et al. 1985b)
- 0.00729 (20°C, supercooled liquid \( S_L \), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.00173, 0.00158, 0.00122, 0.0015 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.00181 (calculated-TSA, Abramowitz & Yalkowsky 1990)
- 0.0024 (calculated-MCI \( \chi \), Patil 1991)
- 0.00151 (calculated-QSPR, Dunnivant et al. 1992)
- 0.00268 (calculated-group contribution method, Kühne et al. 1995)
- 0.00268, 0.0072 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
\[ \log [S_L/(\text{mol/L})] = -1.12 + 1403/(T/K) \] (supercooled liquid, Passivirta et al. 1999)
\[ 6.57 \times 10^{-3} \] (quoted average value from Bidleman 1984, Erickson 1986)
\[ 7.51 \times 10^{-3}, 6.75 \times 10^{-3} \] (supercooled liquid; LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 5.06 \times 10^{-4}, 5.65 \times 10^{-4} (supercooled liquid \( P_L \), GC-RT correlation, different stationary phases, Bidleman 1984)
- 1.58 \times 10^{-4} (GC-R1 correlation, Burkhard et al. 1985a)
- 4.87 \times 10^{-4} (supercooled liquid \( P_L \), GC-R1 correlation, Burkhard et al. 1985b)
- 5.10 \times 10^{-4}, 4.96 \times 10^{-4} (supercooled liquid \( P_L \), GC-R1 correlation, different stationary phases, Foreman & Bidleman 1985)
- 5.33 \times 10^{-4} (quoted average value from Bidleman 1984, Erickson 1986)
- 1.47 \times 10^{-4} (20°C, supercooled liquid \( P_L \), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
\[ \log (P/\text{mmHg}) = 11.60 - 5040/(T/K) \] (GC-RT correlation, Tateya et al. 1988)
3.31 × 10⁻⁴, 4.90 × 10⁻⁴ (supercooled liquid Pₗ, GC-RI correlation, different stationary phases, Fischer et al. 1992)

\[
\log (P/P_\text{Pa}) = -4800/(T/K) + 12.81
\]

(20°C, supercooled liquid Pₗ, GC-RT correlation, Falconer & Bidleman 1994)

3.63 × 10⁻⁴ (solid, supercooled liquid, Passivirta et al. 1999)

\[
\log (P/P_\text{Pa}) = 15.76 - 5842/(T/K)
\]

(solid, Passivirta et al. 1999)

5.37 × 10⁻⁴; 5.62 × 10⁻⁴ (supercooled liquid Pₗ, Fischer et al. 1992)


3.63 × 10⁻⁴ (solid, supercooled liquid, Passivirta et al. 1999)

\[
\log (P/P_\text{Pa}) = -5034/(T/K) + 13.62
\]

(solid, LDV linear regression of literature data, Li et al. 2003)

\[
\log (P/P_\text{Pa}) = -4770/(T/K) + 12.75
\]

(supercooled liquid, FA V final adjusted eq., Li et al. 2003)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

48.64 (calculated-P/C, Murphy et al. 1983)

11.04 (calculated-P/C, Burkhard et al. 1985b)

7.60 (20°C, calculated-P/C, Murphy et al. 1987)

10.84 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)

2.13 (wetted-wall column-GC, Brunner et al. 1990)

69.0 (Wittlinger & Ballschmiter 1990)

13.17 (calculated-QSPR, Dunnivant et al. 1992)

\[
\log \left[ \frac{H}{(\text{mol} \cdot \text{m}^3/\text{Pa})} \right] = 13.93 - 3757/(T/K)
\]

(Passivirta et al. 1999)

44.6± 1.7 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)

ln \( K_{\text{AW}} \) = 31.152 – 10476.3/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

\[
K_{\text{AW}} = \exp\left[-(87.1/(\text{kJ mol}^{-1})/RT + (0.259/(\text{kJ mol}^{-1} \cdot \text{K}^{-1}))/R\right] \text{ where } R = 8.314 \text{ J mol}^{-1} \cdot \text{K}^{-1}
\]


39.81, 30.2 (LDV literature-derived value, FA V final adjusted value, Li et al. 2003)

\[
\log \left[ \frac{H}{(\text{mol} \cdot \text{m}^3/\text{Pa})} \right] = -4672/(T/K) + 17.27
\]

(LDV linear regression of literature data, Li et al. 2003)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):

7.90 (HPLC-RT correlation, Shaw & Connell 1982)


6.67, 6.77, 6.73, 6.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.04, 6.80, 6.84, 6.79 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.42 (average, generator column-GC, Larsen et al. 1992)

6.92 (recommended, Sangster 1993)

7.25 (recommended, Hansch et al. 1995)

7.00, 7.22 (LDV literature-derived value, FA V final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \) at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:


\[
\log K_{\text{OA}} = -5.57 + 4584/(T/K); \text{ temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)}
\]

9.51; 9.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

\[
K_{\text{OA}} = \exp[-(87.1/(\text{kJ mol}^{-1})/RT + (0.259/(\text{kJ mol}^{-1} \cdot \text{K}^{-1}))/R]; \text{ where } R = 8.314 \text{ J mol}^{-1} \cdot \text{K}^{-1}
\]

and temp range: 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

10.62 (10°C, estimated, Thomas et al. 1998)

11.34, 10.20; 10.18 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

10.09 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

9.76, 9.66 (LDV literature derived value, FA V final adjusted value, Li et al. 2003)
Polychlorinated Biphenyls (PCBs)

\[
\log K_{OA} = 4509/(T/K) - 5.37 \quad \text{(LDV linear regression of literature data, Li et al. 2003)}
\]
\[
\log K_{OA} = 4510/(T/K) - 5.47 \quad \text{(FAV final adjusted eq., Li et al. 2003)}
\]

Bioconcentration Factor, \(\log BCF\):
- 5.88; 7.41 (zebrafish: \(\log BCF_w\) wet wt basis; \(\log BCF_l\) lipid wt basis, Fox et al. 1994)
- 3.31–5.47 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.79–5.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 5.88, 7.42 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.42, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, \(\log K_p\) or \(\log K_d\):
- 5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.70 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.52–5.89 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, \(\log K_{OC}\) at 25°C or as indicated:
- 6.49 (suspended particulate matter, calculated-\(K_{OW}\), Burkhard 1984)
- 5.8–7.3, 6.6 (suspended sediment, average, Oliver 1987a)
- 7.60 (algae > 50 \(\mu m\), Oliver 1987a)
- 6.65 (Lake Michigan water column, Swackhamer & Armstrong 1987)
- 5.21, 5.22, 5.17, 4.60 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient \(\log K_a\), Lara & Ernst 1989)
- 5.207, 5.241 (marine humic substances, quoted, calculated-MCI \(\chi\), reported as \(\log K_a\) at 5 mg/L DOC, Sabljic et al. 1989)
- 5.93 (soil from Ispra, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
- 6.50 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 6.50 (soil, calculated-\(K_{OW}\), Girvin & Scott 1997)
- 6.04–7.28; 5.80–7.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.51; 6.28, 6.78, 6.41 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 6.27–7.44 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):

Volatileization:
Photolysis: photodegradation rate constant \(k = (0.08 \pm 0.01)\) h\(^{-1}\) with \(t_{1/2} = 8.2\) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).
Oxidation: rate constant \(k\) for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO\(_3\) radical and \(k_{O3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:
\[
k_{OH}(\text{calc}) = (0.16–0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\] for hexachlorobiphenyls, and the tropospheric lifetime \(\tau(\text{calc}) = 29–60\) d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \(k_1\) and Elimination \(k_2\) Rate Constants:
- \(k_1 = 0.049\) h\(^{-1}\); \(k_2 = 0.008\) h\(^{-1}\) (mayfly-sediment model II, Gobas et al. 1989)
- \(k_1 = 4770\) d\(^{-1}\); \(k_2 = 0.00624\) d\(^{-1}\) (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- \(k_1 = 0.0344\) d\(^{-1}\) with an elimination \(t_{1/2} = 20.2\) d (earthworm, Belfroid et al. 1995)
- \(k_1 = 0.005\) d\(^{-1}\) with \(t_{1/2} = 139\) d and \(k_2 = 0.011\) d\(^{-1}\) with \(t_{1/2} = 64\) d for food concn of 31 ng/g and 176 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- \(k_1 = 0.00226\) h\(^{-1}\); \(k_2 = 0.145\) h\(^{-1}\) (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 5 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.05 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with t_1/2 = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with t_1/2 = 191 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);

t_1/2 = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation t_1/2 = (8.2 ± 0.3) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

t_1/2 = 120000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: t_1/2 = 19–25 yr (Geyer et al. 2000)

t_1/2 = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: t_1/2 = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination t_1/2 = of 20 d from earthworm (Belfroid et al. 1995)

Depuration t_1/2 = 64–139 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

t_1/2 = 4.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination t_1/2 = 13 d in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration t_1/2 = 186 d for high-dose treatment, t_1/2 = 191 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
TABLE 7.1.1.138.1
Reported Henry’s law constants and octanol-air partition coefficients of 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>4</td>
<td>2.88</td>
</tr>
<tr>
<td>11</td>
<td>7.50</td>
</tr>
<tr>
<td>18</td>
<td>18.68</td>
</tr>
<tr>
<td>25</td>
<td>44.6</td>
</tr>
<tr>
<td>31</td>
<td>91.1</td>
</tr>
</tbody>
</table>

enthalpy, entropy change:

$\Delta H_{OA}/(kJ \cdot mol^{-1}) = 87.77$
$\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 259 \pm 26$

$\ln K_{AW} = -\Delta H/RT + \Delta S/R$

A 31.1523

$\log K_{OA} = A + B/T$

A $-5.17$

B 4380

FIGURE 7.1.1.138.1 Logarithm of Henry’s law constant and $K_{OA}$ versus reciprocal temperature for 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138).
7.1.1.139 2,2′,3,4,4′,6-Hexachlorobiphenyl (PCB-139)

Common Name: 2,2′,3,4,4′,6-Hexachlorobiphenyl
Synonym: PCB-139
Chemical Name: 2,2′,3,4,4′,6-hexachlorobiphenyl
CAS Registry No: 56030-56-9
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
123 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0126 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.05 × 10⁻³ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.65 × 10⁻¹, 3.30 × 10⁻¹, 2.33 × 10⁻¹ (P₁ supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.26 × 10⁻³ (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)
log (P₁/Pa) = –4681/(T/K) + 12.78 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
87.24 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.32 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₐₖ = –ΔHₚ/RT + ΔSₚ/R; R is the ideal gas constant, ΔHₚ = 47 ± 8 kJ/mol, ΔSₚ = 0.13 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₐₖ:
6.79 (calculated-TSA, Burkhard 1984)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.12, 6.68; 6.54, 6.50 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.70 (recommended, Sangster 1993)
6.95 (recommended, Hansch et al. 1995)
6.6419 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₐₐ:
10.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.59 (suspended particulate matter, Burkhard 1984)
- 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12} \text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \text{d at room temp.}$ (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.140 2,2',3,4,4',6'-Hexachlorobiphenyl (PCB-140)

![Chemical Structure](image)

Common Name: 2,2',3,4,4',6'-Hexachlorobiphenyl  
Synonym: PCB-140, 2,2',3,4,4',6'-hexachloro-1,1'-biphenyl  
Chemical Name: 2,2',3,4,4',6'-hexachlorobiphenyl  
CAS Registry No: 59291-64-4  
Molecular Formula: C$_{12}$H$_4$Cl$_6$  
Molecular Weight: 360.878  
Melting Point (°C): 123  
(estimated, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm$^3$):  
Molar Volume (cm$^3$/mol): 310.0  
(calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{fus}$ = 56 J/mol K), F:  
Water Solubility (g/m$^3$ or mg/L at 25°C):  
0.0125  
($S_L$ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00314, 0.00203, 0.0015, 0.00194 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
0.00228  
(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
0.00325  
(calculated-QSPR, Dunnivant et al. 1992)  
Vapor Pressure (Pa at 25°C):  
1.26 × 10$^{-3}$  
($P_L$ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00138  
(GC-RI correlation, Burkhard et al. 1985b)  
Henry’s Law Constant (Pa·m$^3$/mol at 25°C):  
36.38  
(calculated-P/C, Burkhard 1984)  
43.06  
(calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)  
31.17  
(calculated-QSAR, Dunnivant et al. 1992)  
68.8  
(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\[
\ln K_{AW} = -\frac{\Delta H_R}{RT} + \frac{\Delta S_R}{R}; \quad R \text{ is the ideal gas constant, } \Delta H_R = 47 \pm 8 \text{ kJ/mol, } \Delta S_R = 0.13 \pm 0.03 \text{ kJ/mol·K (Bamford et al. 2002)}—\text{see Comment by Goss et al. 2004}
\]  
Octanol/Water Partition Coefficient, log $K_{ow}$:  
6.79  
(calculated-TSA, Burkhard 1984)  
6.48, 6.70, 6.47, 6.66 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
6.67  
(calculated-TSA, Hawker & Connell 1988a)  
7.01, 6.86; 6.56, 6.51 (multicolumn HPLC-$k'$ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)  
6.58  
(recommended, Sangster 1993).  
6.97  
(recommended, Hansch et al. 1995)  
6.4851  
(calculated-molecular properties MNDO-AM1 method, Makino 1998)  
Octanol/Air Partition Coefficient, log $K_{oa}$:  
9.91  
(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.59 (suspended particulate matter, Burkhard 1984)
- 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \text{ d at room temp.}$ (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
### 7.1.1.141 2,2′,3,4,5,5′-Hexachlorobiphenyl (PCB-141)

![Chemical Structure](image)

**Common Name:** 2,2′,3,4,5,5′-Hexachlorobiphenyl  
**Synonym:** PCB-141, 2,2′,3,4,5,5′-hexachloro-1,1′-biphenyl  
**Chemical Name:** 2,2′,3,4,5,5′-hexachlorobiphenyl  
**CAS Registry No:** 52712-04-6  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{4}Cl\textsubscript{6}  
**Molecular Weight:** 360.878

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>85 (Kühne et al. 1995; Ruelle &amp; Kesselring 1997)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm\textsuperscript{3})</td>
<td></td>
</tr>
</tbody>
</table>
| Molar Volume (cm\textsuperscript{3}/mol)      | 310.0 (calculated-Le Bas method at normal boiling point)  
                                             | 237.4 (Ruelle & Kesselring 1997) |
| Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol) |                                            |
| Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K)  |                                            |
| Fugacity Ratio at 25°C (assuming ΔS\textsubscript{fus} = 56 J/mol K), F: 0.258 (mp at 85°C) |                                            |
| Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated) | 0.0160 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
                                            | 0.00755 (20°C, supercooled liquid, Murphy et al. 1987)  
                                            | 0.00109, 0.00150, 0.00134, 0.00165 (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)  
                                            | 0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
                                            | 0.0025 (calculated-group contribution method, Kühne et al. 1995)  
                                            | 0.00244, 0.00642 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997) |
| Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations) | 2.73 × 10\textsuperscript{-3} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
                                            | 0.00295 (GC-Rl correlation, Burkhard et al. 1985b)  
                                            | 2.05 × 10\textsuperscript{-4} (20°C, supercooled liquid, Murphy et al. 1987)  
                                            | log (P/mmHg) = 11.50 – 5080/(T/K) (GC-RT correlation, Tateya et al. 1988)  
                                            | 5.01 × 10\textsuperscript{-4}, 6.46 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)  
                                            | log (P\textsubscript{L}/P\textsubscript{A}) = –4816/(T/K) + 12.94 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994) |
| Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C): | 61.5 (calculated-P/C, Burkhard 1984)  
                                            | 9.83 (20°C,calculated-P/C, Murphy et al. 1987)  
                                            | 14.49 (calculated-QSAR-MCl \chi, Šabljić & Güsten 1989)  
                                            | 2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)  
                                            | 17.61 (calculated-QSPR, Dunnivant et al. 1992)  
                                            | 6.54 (calculated-QSPR, Achman et al. 1993)  
                                            | 12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
                                            | 54.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
| ln K\textsubscript{AW} = –ΔH\textsubscript{f}/RT + ΔS\textsubscript{f}/R; R is the ideal gas constant, ΔH\textsubscript{f} = 70 ± 7 kJ/mol, ΔS\textsubscript{f} = 0.20 ± 0.03 kJ/mol-K  
                                            | (Bamford et al. 2002)—see Comment by Goss et al. 2004 |
Polychlorinated Biphenyls (PCBs)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 6.69 (calculated-TSA, Burkhard 1984)
- 6.80, 6.79, 6.79, 6.71 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmitter 1988)
- 6.82 (calculated-TSA, Hawker & Connell 1988a)
- 6.98, 7.02; 6.78, 6.73 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.75 (recommended, Sangster 1993)
- 9.538 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 7.19 (recommended, Hansch et al. 1995)
- 7.10, 6.64–6.89 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
- 6.70 (estimated, Girvin & Scott 1997)
- 6.8226 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:
- 10.55 (10°C, estimated, Thomas et al. 1998)
- 11.18, 10.07; 10.13 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \) or \( \log K_p \):
- 5.81; 7.34 (zebrafish: \( \log BCF_W \) wet wt basis; \( \log BCF_L \) lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, \( \log K_p \) or \( \log K_d \):
- 5.80, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, \( \log K_{OC} \):
- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient \( \log K_a \), calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.05 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 6.20 (soil-organic carbon, calculated-\( K_{OW} \) Girvin & Scott 1997)
- 6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcıoğlu 1996)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatileization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3 or as indicated, *data at other temperatures see reference:
\[
k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for hexachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 29–60 \text{ d at room temp.} \text{ (Kwok et al. 1995)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
- \( k_1 = 4910 \text{ d}^{-1} \) (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- \( k_2 = 0.00764 \text{ d}^{-1} \) (22°C, zebrafish, 30-d clearance, Fox et al. 1994)
- \( k_2 = 0.004 \text{ d}^{-1} \) with \( t_{1/2} = 171 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.004 \text{ d}^{-1} \) with \( t_{1/2} = 198 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Half-Lives in the Environment:
   Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
   Surface water:
   Ground water:
   Sediment:
   Soil:
   Biota: depuration $t_{1/2} = 171$ d for high-dose treatment, $t_{1/2} = 198$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.142  2,2′,3,4,5,6-Hexachlorobiphenyl (PCB-142)

Common Name: 2,2′,3,4,5,6-Hexachlorobiphenyl  
Synonym: PCB-142, 2,2′,3,4,5,6-hexachloro-1,1′-biphenyl  
Chemical Name: 2,2′,3,4,5,6-hexachlorobiphenyl  
CAS Registry No: 41411-61-4  
Molecular Formula: C_{12}H_{4}Cl_{6}  
Molecular Weight: 360.878  
Melting Point (°C):  
136.0  (Burkhard et al. 1985b)  
Boiling Point (°C):  
Density (g/cm³):  
310.0  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):  
Entropy of Fusion, ∆S_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.0815 (mp at 136°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
0.0171  (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00361  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
0.000138  (calculated-QSPR, Dunnivant et al. 1992)  
Vapor Pressure (Pa at 25°C):  
3.41 × 10⁻³  (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.000293  (GC-RI correlation, Burkhard et al. 1985b)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
71.74  (calculated-P/C, Burkhard 1984)  
21.18  (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)  
31.89  (calculated-QSPR, Dunnivant et al. 1992)  
68.8  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
ln K_{AW} = -\Delta H_/R + \Delta S_/R; R is the ideal gas constant, ∆H_{fus} = 47 ± 8 kJ/mol, ∆S_{fus} = 0.13 ± 0.03 kJ/mol-K  
(calculated-molecular properties MNDO-AMI method, Makino 1998)  
Octanol/Water Partition Coefficient, log K_{ow}:  
6.66  (calculated-TSA, Burkhard 1984)  
6.51  (calculated-TSA, Hawker & Connell 1988)  
6.94, 6.75; 6.56, 6.41  (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)  
6.85  (recommended, Sangster 1993)  
6.97  (recommended, Hansch et al. 1995)  
6.5729  (calculated-molecular properties MNDO-AMI method, Makino 1998)  
Octanol/Air Partition Coefficient, log K_{oa}:  
9.84  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)  
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, $\log K_{OC}$:

- 6.46 (suspended particulate matter, Burkhard 1984)
- 5.119 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_A$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(\text{calc}) = (0.16–0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.143 2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-143)

Common Name: 2,2',3,4,5,6'-Hexachlorobiphenyl
Synonym: PCB-143, 2,2',3,4,5,6'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,5,6'-hexachlorobiphenyl
CAS Registry No: 68194-15-0
Molecular Formula: C_{12}H_4Cl_6
Molecular Weight: 360.878

Melting Point (°C): 116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0143 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00287, 0.00238, 0.00250, 0.00293 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.046 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.41 × 10⁻³ (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)
9.014 × 10⁻⁴, 9.59 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
7.41 × 10⁻⁴, 1.35 × 10⁻³ (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4681/(T/K) + 12.65 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
127.7 (calculated-P/C, Burkhard 1984)
25.94 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.95 (wetted wall column-GC/ECD, Brunner et al. 1990)
29.83 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (Bamford et al. 2002)
ln K_{AW} = –ΔH_{if}/RT + ΔS_{if}/R; R is the ideal gas constant, ΔH_{if} = 47 ± 9 kJ/mol, ΔS_{if} = 0.13 ± 0.03 kJ/mol K (Bamford et al. 2002) — see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{ow}:
6.74 (calculated-TSA, Burkhard 1984)
6.52, 6.65, 6.51, 6.55 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.60 (calculated-TSA, Hawker & Connell 1988)
6.89, 6.63; 6.51, 6.48 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
Octanol/Air Partition Coefficient, log $K_{OA}$:
- 6.56 (recommended, Sangster 1993)
- 6.92 (recommended, Hansch et al. 1995)
- 6.545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.54 (suspended particulate matter, Burkhard 1984)
- 5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29$–$60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$$k_1 = 3 \text{ (food lipid mg)/(g worm lipid-d)}; k_2 = 0.07 \text{ d}^{-1}$$

(earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 10$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.144 2,2',3,4,5',6-Hexachlorobiphenyl (PCB-144)

Common Name: 2,2',3,4,5',6-Hexachlorobiphenyl
Synonym: PCB-144, 2,2',3,4,5',6-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,5',6-hexachlorobiphenyl
CAS Registry No: 68194-14-9
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C): 110 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hᵥus (kJ/mol):
Entropy of Fusion, ∆Sᵥus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sᵥus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0126 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01294 (20°C, supercooled liquid, Murphy et al. 1987)
0.00353 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.45 × 10⁻³ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00371 (GC-RI correlation, Burkhard et al. 1985b)
5.07 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
0.00166, 0.00105 (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P₁/Pa) = –4681/(T/K) + 12.70 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
98.23 (calculated-P/C, Burkhard 1984)
14.19 (20°C, calculated-P/C, Murphy et al. 1987)
32.22 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
5.70 (calculated-QSPR, Achman et al. 1993)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K₄ₐₖ = –∆Hユー/RT + ∆Sユー/R; R is the ideal gas constant, ∆Hユー = 47 ± 8 kJ/mol, ∆Sユー = 0.13 ± 0.03 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₒₐₖ:
6.79 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a, 1990)
6.96, 6.68; 6.38, 6.29 (multi-column HPLC-k correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.45 (recommended, Sangster 1993)
6.79 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

- 10.73, 9.62; 9.62 (0, 20°C, multi-column GC-k’ correlation; calc at 20°C, Zhang et al. 1999)
- 10.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{Bi}$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.59 (suspended particulate matter, Burkhard 1984)
- 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.20 (soil-organic carbon, calculated-$K_{OW}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12} \, \text{cm}^3 \, \text{molecule}^{-1} \, \text{s}^{-1}$$
for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \, \text{d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_2 = 0.005 \, \text{d}^{-1}$ with $t_{1/2} = 137 \, \text{d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \, \text{d}^{-1}$ with $t_{1/2} = 184 \, \text{d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 137 \, \text{d}$ for high-dose treatment, $t_{1/2} = 184 \, \text{d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.145 2,2',3,4,6,6'-Hexachlorobiphenyl (PCB-145)

![ Chemical Structure Image ]

Common Name: 2,2',3,4,6,6'-Hexachlorobiphenyl
Synonym: PCB-145, 2,2',3,4,6,6'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,6,6'-hexachlorobiphenyl
CAS Registry No: 74472-40-5
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878

Melting Point (°C):
84 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
310.0 (calculated-Le Bas method)

Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), \( F \):

Water Solubility (g/m³ or mg/L at 25°C):
0.0137 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.36 \times 10⁻³ (\( Pₗ \) supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681 (GC-RI correlation, Burkhard et al. 1985b)
0.00309 (supercooled liquid \( Pₗ \), GC-RI correlation, Fischer et al. 1992)
log (\( Pₗ/Pa \)) = –4303/T + 11.90 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
168.2 (calculated-P/C, Burkhard 1984)
41.34 (calculated-QSPR-MCI \( \chi \), Sabljic & Güsten 1989)
46.61 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln \( K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R \); \( R \) is the ideal gas constant, \( \Delta H_{f} = 27 \pm 5 \) kJ/mol, \( \Delta S_{f} = 0.06 \pm 0.02 \) kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):
6.76 (calculated-TSA, Burkhard 1984)
6.25 (calculated-TSA, Hawker & Connell 1988a)
6.92, 6.59; 6.30, 6.26 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phase, Risby et al. 1990)
6.28, 6.78 (quoted average values of Risby et al. 1990, Sangster 1993)
6.71 (recommended, Hansch et al. 1995)
6.2606 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log \( K_{oa} \):
9.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_D:

Sorption Partition Coefficient, log K_OC:
- 6.56 (suspended particulate matter, Burkhard 1984)
- 4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_a, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:
- Volatilization:
- Photolysis:
- Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO3 radical and k_{O3} with O3 or as indicated, *data at other temperatures see reference: k_{OH(calc)} = (0.16 – 0.5) × 10^{-12} cm^3 molecule^{-1} s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
**7.1.1.146 2,2′,3,4′,5,5′-Hexachlorobiphenyl (PCB-146)**

![Chemical structure of PCB-146](image)

Common Name: 2,2′,3,4′,5,5′-Hexachlorobiphenyl  
Synonym: PCB-146, 2,2′,3,4′,5,5′-hexachloro-1,1′-biphenyl  
Chemical Name: 2,2′,3,4′,5,5′-hexachlorobiphenyl  
CAS Registry No: 51908-16-8  
Molecular Formula: C_{12}H_{4}Cl_{6}  
Molecular Weight: 360.878  
Melting Point (°C):  
90  
Boiling Point (°C):  
Density (g/cm³):  
310.0  
Molar Volume (cm³/mol):  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
0.0141 (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00759 (20°C, supercooled liquid, Murphy et al. 1987)  
0.00095 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)  
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
7.28 × 10⁻⁴ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.000801 (GC-RI correlation, Burkhard et al. 1985b)  
7.73 × 10⁻⁴, 9.614 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
1.87 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)  
6.31 × 10⁻⁴, 8.51 × 10⁻⁴ (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)  
log (P₁/Pa) = –4816/(T/K) + 13.04 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
18.54 (calculated-P/C, Burkhard 1984)  
8.92 (20°C, calculated-P/C, Murphy et al. 1987)  
25.23 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)  
2.53 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)  
19.0 (calculated-QSPR, Dunnivant et al. 1992)  
17.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
60.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)  
ln K_{aw} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 59 ± 7 kJ/mol, ΔS_{f} = 0.17 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log K_{ow}:  
6.74 (calculated-TSA, Burkhard 1984)  
6.85 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)  
6.89 (calculated-TSA, Hawker & Connell 1988a)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
10.96, 9.84 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
9.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Partition Coefficient between particulate and dissolved contaminant concentrations, log $K_P$ or log $K_d$
5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log $K_{OC}$:
6.54 (suspended particulate matter, Burkhard 1984)
5.40 (Lake Superior suspended solids, GC/ECD, Baker et al. 1986)
5.18, 5.22, 5.14, 4.58 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_p$, Lara & Ernst 1989)
5.18; 5.22 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_p$, observed; calculated-MCI $\chi$, Sabljic et al. 1989)
5.87 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (colloids and micro-particulates from precipitation events, Murray & Andren 1992)
6.20 (soil-organic carbon, calculated-K$_{OW}$ Girvin & Scott 1997)
6.01 (soil, calculated-Characteristic Root Index CRI, Şaçan & Balcioğlu 1996)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_1/2$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
\[ k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
\[ k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 166 \text{ d} \] (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
\[ k_2 = 0.003 \text{ d}^{-1} \text{ with } t_{1/2} = 216 \text{ d} \] (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 166$ d for high-dose treatment, $t_{1/2} = 216$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.147 2,2',3,4',5,6-Hexachlorobiphenyl (PCB-147)

Common Name: 2,2',3,4',5,6-Hexachlorobiphenyl
Synonym: PCB-147, 2,2’,3,4’,5,6-hexachloro-1,1’-biphenyl
Chemical Name: 2,2’,3,4’,5,6-hexachlorobiphenyl
CAS Registry No: 68194-13-8
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
   116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
   310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   0.0134 (S₀ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
   0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   2.86 × 10⁻³ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
   0.00309 (GC-RI correlation, Burkhard et al. 1985b)
   log (P/mmHg) = 11.20 – 4910/(T/K) (GC-RT correlation, Tateya et al. 1988)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   77.21 (calculated-P/C, Burkhard 1984)
   32.63 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
   5.17 (wetted wall column-GC/ECD, Brunner et al. 1990)
   31.97 (calculated-QSPR, Dunnivant et al. 1992)
   5.70 (calculated-QSPR, Achman et al. 1993)
   68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
   ln Kₛₜw = −ΔH_w/RT + ΔS_w/R; R is the ideal gas constant, ΔH_w = 47 ± 8 kJ/mol, ΔS_w = 0.13 ± 0.02 kJ/mol-K
   (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₜₜw:
   6.77 (calculated-TSA, Burkhard 1984)
   6.64 (calculated-TSA, Hawker & Connell 1988a)
   7.07, 6.73, 6.52, 6.51 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary
   phases, Risby et al. 1990)
   6.52, 6.90 (quoted average values of Risby et al. 1990, Sangster 1993)
   6.93 (recommended, Hansch et al. 1995)
   6.6069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₜₜ at 25°C or as indicated:
   10.79, 9.672 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
   9.70 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.57 (suspended particulate matter, Burkhard 1984)
- 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:

$$k_{OH} (calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for hexachlorobiphenyls, and the tropospheric lifetime } \tau (calc) = 29\text{–}60 \text{ d at room temp.} \ (Kwok \ et \ al. \ \ 1995)$$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$$k_1 = 0.004 \text{ d}^{-1} \text{ with } t_\frac{1}{2} = 194 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)}$$

$$k_2 = 0.002 \text{ d}^{-1} \text{ with } t_\frac{1}{2} = 283 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)}$$

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_\frac{1}{2} = 194 \text{ d for high-dose treatment, } t_\frac{1}{2} = 283 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)}}$
7.1.1.148 2,2',3,4',5,6'-Hexachlorobiphenyl (PCB-148)

Common Name: 2,2',3,4',5,6'-Hexachlorobiphenyl
Synonym: PCB-148, 2,2',3,4',5,6'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4',5,6'-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C): 104 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0112 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0369 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00204 (GC-RI correlation, Burkhard et al. 1985b)
0.00190, 0.00277 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = –4681/(T/K) + 12.98 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
60.69 (calculated-P/C, Burkhard 1984)
57.65 (calculated-QSPR-MCI χ; Sabljic & Güsten 1989)
43.52 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −∆H_{fus}/RT + ∆S_{fus}/R; R is the ideal gas constant, ∆H_{fus} = 47 ± 8 kJ/mol, ∆S_{fus} = 0.13 ± 0.02 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
6.84 (calculated-TSA, Burkhard 1984)
5.74 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
6.73 (calculated-TSA, Hawker & Connell 1988a)
7.04, 6.74; 6.46, 6.44 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
5.74 (recommended, Sangster 1993)
6.87 (recommended, Hansch et al. 1995)
6.6291 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:

9.51 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

6.64 (suspended particulate matter, Burkhard 1984)

5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

5.707 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volutilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.149 2,2′,3,4′,5′,6-Hexachlorobiphenyl (PCB-149)

Common Name: 2,2′,3,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-149, 2,2′,3,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 38380-04-0
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 369.9
Melting Point (°C):
  oil (Erickson 1986)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 1.0 (Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C):
  0.0127 (Sₗ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.01217 (20°C, supercooled liquid, Murphy et al. 1987)
  0.00414 (RP-HPLC-k’ correlation, Brodsky & Ballschmider 1988)
  0.00454 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  1.124 × 10⁻³, 1.83 × 10⁻³ (Pₗ, supercooled liquid, GC-RT correlation, different stationary phases, Bidleman 1984)
  1.57 × 10⁻³ (Pₗ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  1.72 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985b)
  0.00105, 0.00158 (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  1.47 × 10⁻³ (Pₗ, supercooled liquid, quoted average value of Bidleman 1984, Erickson 1986)
  4.96 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
  8.51 × 10⁻⁴, 1.48 × 10⁻³ (supercooled liquid Pₗ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  log (Pₗ/Pa) = –4689/(T/K) + 12.78 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  44.79 (calculated-P/C, Burkhard 1984)
  15.0 (20°C, calculated-P/C, Murphy et al. 1987)
  22.09 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  4.32 (calculated-QSPR, Achman et al. 1993)
  24.03 (calculated-QSPR, Dunnivant et al. 1992)
  0.682; 1.994 (0, 15°C, Hornbuckle et al. 1994)
  25.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  68.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{ μ}/RT + ΔS_{ μ}/R; R is the ideal gas constant, ΔH_{ μ} = 46 ± 7 kJ/mol, ΔS_{ μ} = 0.12 ± 0.02 kJ/mol·K
  (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
  6.70 (HPLC-RT correlation, Shaw & Connell 1982)
  6.14, 7.28 (RP-HPLC-k’ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.79  (calculated-TSA, Burkhard 1984)
6.41  (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.67  (calculated-TSA, Hawker & Connell 1988a)
7.02, 7.0; 6.45, 6.47 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.54  (generator column-GC, Larsen et al. 1992)
6.41  (recommended, Sangster 1993)
6.86  (recommended, Hansch et al. 1995)
6.4731 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.27; 8.68  (generator column; calculated-K_{OW}/K_{AW}, Kömp & McLachlan 1997a)
log K_{OA} = –6.50 + 4700/(T/K), temp range 10–43°C (Kömp & McLachlan 1997a)
9.27  (quoted, Kömp & McLachlan 1997b)
10.83, 9.74; 9.80 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.78  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{b}:

Biota Sediment Accumulation Factor, BSAF:
105  (trout, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:
6.59  (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_{a}, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.79  (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.10  (colloids and micro-particulates from precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_{3} radical and k_{O3} with O_{3} or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} for hexachlorobiphenyls, and the tropospheric lifetime \tau(calc) = 29–60 \text{ d at room temp.} (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_{1} and k_{2}):
k_{1} = 0.00097 \text{ h}^{-1}; k_{2} = 0.240 \text{ h}^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_{1} = 0.004 \text{ d}^{-1} with t_{1/2} = 162 \text{ d} (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_{2} = 0.003 \text{ d}^{-1} with t_{1/2} = 199 \text{ d} (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration t_{1/2} = 162 \text{ d for high-dose treatment, t_{1/2} = 199 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)}}
7.1.1.150 2,2',3,4',6,6'-Hexachlorobiphenyl (PCB-150)

Common Name: 2,2',3,4',6,6'-Hexachlorobiphenyl
Synonym: PCB-150, 2,2',3,4',6,6'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4',6,6'-hexachlorobiphenyl
CAS Registry No: 68194-08-1
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
104 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0121 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00907 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.07 × 10⁻³ (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00438 (GC-RI correlation, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C):
121.6 (calculated-P/C, Burkhard 1984)
52.18 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln K_{AW} = −ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 27 ± 5 kJ/mol, ΔS_{fus} = 0.06 ± 0.02 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.81 (calculated-TSA, Burkhard 1984)
6.32 (calculated-TSA, Hawker & Connell 1988a)
6.69; 6.59; 6.34, 6.27 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.64, 6.31 (quoted average values of Risby et al. 1990, Sangster 1993)
6.75 (recommended, Hansch et al. 1995)
6.1643 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{Bi}:
Sorption Partition Coefficient, log $K_{OC}$:

- 6.61 (suspended particulate matter, Burkhard 1984)
- 4.924 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for hexachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 29-60 \text{ d at room temp. (Kwok et al. 1995)}$$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.151 2,2',3,5,5',6-Hexachlorobiphenyl (PCB-151)

Common Name: 2,2',3,5,5',6-Hexachlorobiphenyl
Synonym: PCB-151, 2,2',3,5,5',6-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',3,5,5',6-hexachlorobiphenyl
CAS Registry No: 52663-63-5
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
   101 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm³):
   310.0 (calculated-Le Bas method at normal boiling point)
   237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $ΔH_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $ΔS_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $ΔS_{\text{fus}} = 56 J/mol K$), F: 0.180 (mp at 101°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   0.0134 (S_l, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
   0.01355 (20°C, supercooled liquid, Murphy et al. 1987)
   0.00454, 0.00414, 0.00487, 0.00337 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
   0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
   0.00223 (calculated-QSPR, Dunnivant et al. 1992)
   0.00203 (calculated-group contribution method, Kühne et al. 1995)
   0.00173, 0.00454 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
   0.00559 (calculated-mp and K_{ow}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   3.32 × 10⁻³ (P_l, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
   1.16 × 10⁻³, 1.67 × 10⁻⁴, 2.23 × 10⁻⁴ (calculated-MW, GC-RI correlation, MCI χ, Burkhard et al. 1985b)
   0.00177, 0.00255 (supercooled liquid P_l, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
   5.97 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
   log (P/mmHg) = 11.30 – 4910/(T/K) (GC-RT correlation, Tateya et al. 1988)
   1.91 × 10⁻³ (supercooled liquid P_l: GC-RI correlation, Fischer et al. 1992)
   log (P_l/Pa) = –4681/(T/K) + 12.95 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
   86.94 (calculated-P/C, Burkhard 1984)
   15.91 (20°C, calculated-P/C, Murphy et al. 1987)
   52.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
   5.98 (wetted wall column-GC/ECD, Brunner et al. 1990)
   28.69 (calculated-QSPR, Dunnivant et al. 1992)
   33.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
73.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_f/RT + \Delta S_f/R; \]  
R is the ideal gas constant, \( \Delta H_f = 37 \pm 5 \text{ kJ/mol}, \Delta S_f = 0.10 \pm 0.02 \text{ kJ/mol-K} \)  
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 6.76 (calculated-TSA, Burkhard 1984)
- 6.38, 6.49, 6.32, 6.51 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballshmiter 1988)
- 6.64 (calculated-TSA, Hawkner & Connell 1988a)
- 6.95, 7.35; 6.44, 6.43 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.45 (generator column-GC, Larsen et al. 1992)
- 6.43 (recommended, Sangster 1993)
- 6.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C or as indicated:

- 10.08 (10°C, estimated, Thomas et al. 1998)
- 10.68, 9.58 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 9.68 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log \( BCF \) or log \( K_b \):

- 5.54; 7.07 (zebrafish: log \( BCF_W \) wet wt basis; log \( BCF_L \) lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log \( K_{oc} \):

- 6.56 (suspended particulate matter, Burkhard 1984)
- 5.03, 5.11, 5.09, 4.41 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log \( K_a \), Lara & Ernst 1989)
- 5.031; 5.083 (marine humic substances with 5 mg/L DOC, reported as association coefficient log \( K_a \), observed; calculated-MCI \( \chi \), Sabljic et al. 1989)
- 6.05, 6.05, 5.93 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 4.99, 4.82; 4.85 (sediments from Brown’s Lake, Helmet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
- 6.20 (soil-organic carbon, calculated-\( K_{ow} \) Girvin & Scott 1997)
- 5.75 (4.96–6.18) (sediment: organic carbon OC \( \geq 0.5\% \), average, Delle Site 2001)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:

\[ k_{OH}(\text{calc}) = (0.16 – 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for hexachlorobiphenyls, and the tropospheric lifetime } \tau(\text{calc}) = 29–60 \text{ d at room temp.} \text{ (Kwok et al. 1995)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

\[ k_1 = 4220 \text{ d}^{-1}; \ k_2 = 0.0121 \text{ d}^{-1} \text{ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)} \]
\[ k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 174 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)} \]
\[ k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 196 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)} \]
Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 174$ d for high-dose treatment, $t_{1/2} = 196$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.152 2,2’,3,5,6,6’-Hexachlorobiphenyl (PCB-152)

Common Name: 2,2’,3,5,6,6’-Hexachlorobiphenyl
Synonym: PCB-152, 2,2’,3,5,6,6’-hexachloro-1,1’-biphenyl
Chemical Name: 2,2’,3,5,6,6’-hexachlorobiphenyl
CAS Registry No: 68914-09-2
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
111 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0145 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
5.95 × 10⁻³ (P_{T} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00638 (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
147.9 (calculated-P/C, Burkhard 1984)
35.57 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
43.32 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\ln K_{AW} = -ΔH_{f}^{T}/R + ΔS_{f}^{T}/R; R is the ideal gas constant, ΔH_{f} = 27 ± 5 kJ/mol, ΔS_{f} = 0.06 ± 0.02 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
6.73 (calculated-TSA, Burkhard 1984)
6.22 (calculated-TSA, Hawker & Connell 1988a)
6.86, 6.36; 6.10, 6.09 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.61, 6.10 (average values of Risby et al. 1990, Sangster 1993)
6.51 (recommended, Hansch et al. 1995)
6.2295 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
9.44 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{bi}:
Sorption Partition Coefficient, log $K_{OC}$:
- 6.53 (suspended particulate matter, Burkhard 1984)
- 4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH(calc)} = (0.16–0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.153 2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153)

Common Name: 2,2',4,4',5,5'-Hexachlorobiphenyl
Synonym: PCB-153, 2,2',4,4',5,5'-hexachloro-1,1'-biphenyl
Chemical Name: 2,2',4,4',5,5'-hexachlorobiphenyl
CAS Registry No: 35065-27-1
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
103.5 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999; Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH₉₅ (kJ/mol):
20.90 (Oppenhuizen et al. 1987; Ruelle et al. 1993)
17.50 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS₉₅ (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.169 (calculated, assuming ΔS₉₅ = 56 J/mol K, Mackay et al. 1980; Shiu & Mackay 1986)
0.167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0088 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.0012 (generator column-GC/ECD, Weil et al. 1974)
9.53 × 10⁻⁴ (shake flask-GC/ECD, Haque & Schmedding 1975)
9.50 × 10⁻⁴ (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
0.00105 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
6.9 × 10⁻⁵ (calculated-UNIFAC activity coefficients, Banerjee 1985)
0.00914 (20°C, supercooled liquid S₁, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
8.86 × 10⁻⁴, 9.4 × 10⁻⁴, 1.34 × 10⁻³, 1.5 × 10⁻³ (RP-HPLC-k'correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.28 × 10⁻⁵ (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.60 × 10⁻⁴ (generator column-GC/ECD, Dunnivant & Elzerman 1988)
8.45 × 10⁻⁴ (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
4.62 × 10⁻³, 8.45 × 10⁻³, 1.28 × 10⁻² (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
S/(mol/L) = 1.15 × 10⁻⁸ exp(0.028-t°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
log x = −1059/(T/K) − 5.819, temp range 4–40°C, ΔH₅₁ = 20.3 kJ/mol (generator column-GC/ECD, Doucette & Andren 1988a)
0.00115 (22°C, generator column-GC/ECD, Oppenhuizen et al. 1988)
log [S₁/(mol/L)] = −1.20 − 1113/(T/K) (supercooled liquid S₁, Passivirta et al. 1999)
ln x = −13.37313 − 2445.3/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0136, 0.0111 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S₁/(mol m⁻³)] = −1305/(T/K) + 0.14 (supercooled liquid S₁, FAV final adjusted eq., Li et al. 2003)
Polychlorinated Biphenyls (PCBs)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

- $6.80 \times 10^{-4}$, $7.19 \times 10^{-4}$ (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Bidleman 1984)
- $6.63 \times 10^{-3}$ (supercooled liquid $P_L$, GC-RT correlation Burkhard 1984)
- $1.24 \times 10^{-4}$ (GC-RI correlation, Burkhard et al. 1985a)
- $6.63 \times 10^{-4}$ (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
- $7.08 \times 10^{-4}$, $8.13 \times 10^{-4}$ (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- $4.57 \times 10^{-4}$ (supercooled liquid $P_L$, GC-RT correlation, Burkhard et al. 1985b)

Temperature dependence equations:

- $7.0 \times 10^{-4}$ (solid $P_S$, supercooled liquid $P_L$, Shiu & Mackay 1986)
- $2.53 \times 10^{-4}$ (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- $1.19 \times 10^{-4}$; $7.0 \times 10^{-4}$ (selected values: solid $P_S$; supercooled liquid $P_L$, Shiu & Mackay 1986)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

- $35.46$ (calculated, Murphy et al. 1983)
- $12.46$ (gas stripping-GC, Coates 1984)
- $17.93$ (calculated-P/C, Burkhard et al. 1985b)
- $6.08$ (20°C, batch stripping-GC, Oliver 1985)
- $42.9$ (calculated-P/C, Shiu & Mackay 1986)
- $10.03$ (20°C, calculated-P/C, Murphy et al. 1987)
- $50.34$ (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
- $2.33$ (wetted-wall column-GC/ECD, Brunner et al. 1990)
- $16.70$ (calculated-QSIMP, Dunnivant et al. 1992)
- $13.98 \pm 1.5, 13.48 \pm 1.2$ (gas stripping-GC/ECD, purge vessel’s height at 26-cm; 67-cm; Girvin et al. 1997)

Octanol/Water Partition Coefficient, log $K_{OW}$:

- $6.72$ (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
- $8.35$ (Hansch & Leo 1979)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.50  
10.04*  

$\log K_{OA} = -6.02 + 4696/(T/K)$; temp range –10 to +30°C (generator column-GC, Harner & Bidleman 1996)

9.37; 9.09  

$\log K_{OA} = -5.49 + 4430/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

9.52, 9.44  

$\log K_{OA} = 4966/(T/K) – 7.14$ (LDV linear regression of literature data, Li et al. 2003)

$\log K_{OA} = 3785/(T/K) – 7.00$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

4.68 (oyster, Vreeland 1974)

4.66 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)

4.48, 5.23 (calculated-S, $K_{SC}$, Kenaga 1980)

5.23, 3.76 (amphipods, clams, Lynch et al. 1982)

5.03, 4.88, 4.65 (algae, snail, aquatic earthworm, Lynch et al. 1982)

4.82, 4.63 (crayfish, fish, Lynch et al. 1982)

4.00, 4.72, 3.77 (calculated-S, calculated-C, calculated-$K_{OW}$, Lynch et al. 1982)

0.99 (poultry, Garten & Trabalka 1983)

6.78 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984)

4.84 (rainbow trout, ratio of uptake and depuration rate constants, Muir et al. 1985)

5.87; 6.00 (rainbow trout: laboratory studies; Lake Ontario field data, Oliver & Niimi 1985)

2.60, 2.48 (human fat of lipid, wet wt. basis, calculated-$K_{OW}$, Geyer et al. 1987)

5.32 (guppy, Gobas et al. 1987)

4.57 ($Selenastrum capricornutum$, Mailhot 1987)

4.48 (worms, Oliver 1987c)

4.84, 5.32 (fish, calculated-$C_p/C_w$ or $k_1/k_2$, Connell & Hawker 1988; Hawker 1990)
Polychlorinated Biphenyls (PCBs)

3.85 \( (Hexagenia\ limbata,\ 4^\circ C,\ rate\ const.\ ratio:\ uptake\ and\ depuration\ k_1/k_2,\ Landrum\ &\ Poore\ 1988) \)

4.94–5.28 \( (Hexagenia\ limbata,\ May-November,\ calculated-lipid-normalized,\ Landrum\ &\ Poore\ 1988) \)

5.01 \( (Pontoporeia\ hoyi,\ calculated,\ Evans\ &\ Landrum\ 1989) \)

5.06 \( (guppy,\ estimated,\ Banerjee\ &\ Baughman\ 1991) \)

5.65–7.18 \( (22^\circ C,\ zebrafish:\ log\ BCF_{w,}\ wet\ wt\ basis;\ log\ BCF_{L,}\ lipid\ wt\ basis,\ Fox\ et\ al.\ 1994) \)

3.31–5.57 \( (\text{various marine species, mean dry wt. BCF, Hope et al.} 1998) \)

5.11–6.96 \( (\text{various marine species, mean lipid-normalized BCF, Hope et al.} 1998) \)

3.52 \( (\text{Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al.} 1999) \)

4.68, 5.93 \( (\text{oyster: wet wt basis, lipid wt basis, Geyer et al.} 2000) \)

4.58, 7.40 \( (\text{mussel: wet wt basis, lipid wt basis, Geyer et al.} 2000) \)

5.63, 6.99 \( (\text{guppy: wet wt basis, lipid wt basis, Geyer et al.} 2000) \)

5.65, 7.19 \( (\text{zebrafish: wet wt basis, lipid wt basis, Geyer et al.} 2000) \)

3.95; 3.95 \( (\text{Oncorhynchus mykiss, wet wt basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al.} 2001) \)

4.40 \( (\text{estimated-EPIWIN v3.04, Hardy} 2002) \)

Sorption Partition Coefficient, log \( K_p \): 3.95–4.17 \( (\text{Saginaw Bay sediment, sorption isotherm, Horzempa & Di Toro} 1983) \)

4.12–4.55 \( (\text{Saginaw Bay suspended solids, sorption isotherm, Horzempa & Di Toro} 1983) \)

5.30 \( (\text{Lake Superior suspended solids, field measurement-GC/ECD, Baker et al.} 1986) \)

5.60 \( (\text{average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren} 1992) \)

5.65–5.91 \( (\text{field-generated particulates, New Bedford Harbor, Bergen et al.} 1993) \)

Sorption Partition Coefficient, log \( K_{OC} \) at 25°C or as indicated: 5.62 \( (\text{soil/sediment, batch equilibrium-sorption isotherm, Haque & Schmedding} 1976) \)

5.34 \( (\text{soil, batch equilibrium-sorption isotherm measurement, Chiou et al.} 1979) \)

6.51 \( (\text{soil, calculated-} K_{OW},\ Karickhoff et al.} 1979) \)

6.08 \( (\text{soil, quoted experimental value, Kenaga} 1980) \)

5.33 \( (\text{calculated-} K_{OW},\ Schwarzzenbach & Westall} 1981) \)

6.51 \( (\text{calculated-} K_{OW},\ Schwarzzenbach & Westall 1981 from Karickhoff} 1981) \)

6.43, 6.42, 5.33 \( (\text{calculated-} K_{OW},\ \text{calculated-} C_{L}\text{, calculated-} C_{S},\ Karickhoff} 1981) \)

6.51 \( (\text{sediment, calculated-} K_{OW},\ Lynch et al.} 1982) \)

5.67 \( (\text{suspended particulate matter, calculated-} K_{OW},\ Burkhard} 1984) \)

5.60; 5.50; 7.30 \( (\text{field data of sediment trap material; Niagara River-org. matter; calculated-} K_{OW},\ Oliver & Charlton} 1984) \)

6.61 \( (\text{sediment/pore water-Saginaw Bay, dual radio-tag experiment, Di Toro et al.} 1985) \)

5.51 \( (\text{Aldrich humic acid, reversed phase separation, Landrum et al.} 1985) \)

5.40, 5.70, 6.10 \( (\text{Offshore Grand Haven sediment, nearshore Grand Haven sediment, Benton Harbor sediment, by batch equilibrium-sorption isotherm, Voice & Weber} 1985) \)

7.56, 7.68 \( (\text{river sediment, Coates & Elzerman} 1986) \)

5.575 \( (\text{correlated literature values in soils, Sklarew & Girvin} 1987) \)

5.8–7.3, 6.60; 7.20 \( (\text{suspended sediment, average; algae > 50 µm, Oliver} 1987a) \)

6.60 \( (\text{river sediment 7–13% OC, batch equilibrium, Oliver} 1987) \)

6.48 \( (\text{Lake Michigan water column, Swackhamer & Armstrong} 1987) \)

4.75 \( (\text{12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans} 1988) \)

5.26, 5.25, 5.19, 4.62 \( (\text{humic substances, in concentration of 5, 10, 20, 40 mg/L DOC, reported as log} K_{OC},\ Lara & Ernst} 1989) \)

5.258, 5.222 \( (\text{marine humic substances, calculated-MCI χ, reported as log} K_{OC} \text{ at concentration of 5 mg/L DOC, Sabljic et al.} 1989) \)

6.76, 4.42 \( (\text{Great Lake suspended matter, Great Lake DOC: reversed phase separation, Eadie et al.} 1990) \)

6.18, 6.13, 5.99 \( (\text{North Sea sediments, batch equilibrium, Lara & Ernst} 1990) \)

5.86 \( (\text{Ispra soil, shake flask-GC, Paya-Perez et al.} 1991; quoted, Baker et al.} 2000) \)

6.40 \( (\text{average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren} 1992) \)

5.54 \( (\text{Red Hood sediment, batch equilibrium, Brannon et al.} 1995) \)
5.65 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.42–6.48 (Catlin silt loam, $f_{OC} = 0.0226$, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.77–6.84 (Cloudland loam, $f_{OC} = 0.0024$, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.43–6.52 (Kenoma silt loam, $f_{OC} = 0.0153$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.51–6.57 (Kenoma silt loam, $f_{OC} = 0.0092$, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.19–6.28 (Norborne silt loam, $f_{OC} = 0.0137$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.55 (Norborne silt loam, $f_{OC} = 0.009$, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.41–6.59 (Norborne silt loam, $f_{OC} = 0.0057$, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.40 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
6.20; 5.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.86, 5.81 (sediments: organic carbon $OC$ –0.1%, $OC$ –0.5%, average, Delle Site 2001)
6.05–7.27; 5.30–7.60 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.55; 6.17, 6.96, 6.50 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
5.088 (estimated-EPIWIN v3.04, Hardy 2002)
6.20–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log $K_{OM}$:
4.42 (natural sediment, Eadie et al. 1990)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:
Volatilization: depletion rate constant $k = 17$ d$^{-1}$ from a 26-cm or 67-cm high purge vessel (Girvin et al. 1997);
t$_{1/2}$ = 2.096 d from river, t$_{1/2}$ = 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16–0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 29.5$ d$^{-1}$ in pond, $k_1 = 14.6$ d$^{-1}$ in river, $k_1 = 36.8$ d$^{-1}$ in sand by $Chironomus$ $tentans$ larvae (Muir et al. 1983)

$k_2 = 0.0029$ d$^{-1}$ with elimination $t_2 = 241$ h in pond-sediment, $k_2 = 0.0059$ d$^{-1}$ with $t_2 = 117$ h in river water, $k_2 = 0.0034$ d$^{-1}$ with $t_2 = 203$ h in river sediment and $k_2 = 0.0030$ d$^{-1}$ with $t_2 = 230$ h in sand-sediment by $Chironomus$ $tentans$ larvae (Muir et al. 1983)

$k_2 > 0.0007$ d$^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 800$ d$^{-1}$; $k_2 = 0.004$ d$^{-1}$ (guppy, Bruggeman et al. 1984)
$k_1 = 461$ d$^{-1}$; $k_2 = 0.008$ d$^{-1}$ (rainbow trout, total $^{14}$C in whole fish-wet weight, Muir et al. 1985)
$k_1 = 1100$ d$^{-1}$ (guppy, Oppenhuizen 1986)

$k_1 = 63.2$ h$^{-1}$; $k_2 = 0.009$ h$^{-1}$ (10–20°C, $Hexagenia$ $limbata$, Landrum & Poore 1988)
$k_1 = 0.049$ h$^{-1}$; $k_2 = 0.009$ h$^{-1}$ (uptake, depuration of mayfly-sediment model II, Gobas et al. 1989)

$k_1 = 5.7$ L d$^{-1}$ g$^{-1}$; $k_2 = 0.027$ d$^{-1}$ (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

$k_1 = 0.00231$ h$^{-1}$; $k_2 = 0.137$ h$^{-1}$ (in blood plasma of ring doves, Drouillard & Norstrom 2000)
Polychlorinated Biphenyls (PCBs)

$k_1 = 5 \text{ (food lipid mg)/(g worm lipid-d); } k_2 = 0.04 \text{ d}^{-1} \text{ (earthworm, Wågman et al. 2001)}$
$k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 177 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)}$
$k_2 = 0.003 \text{ d}^{-1} \text{ with } t_{1/2} = 219 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)}$
$k_2 = 0.015 \text{ d}^{-1} \text{ with } t_{1/2} = 46.2 \text{ d (juvenile carp in 100-d experiment Stapleton et al. 2004)}$

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radical for hexachlorobiphenyls (Kwok et al. 1995);
$t_{1/2} = 6000 \text{ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)}$.

Surface water: 25–53 min in aqueous solution purged at a flow rate of 1 L/min (Coates 1984);
$t_{1/2} = 123000 \text{ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000); volatilization } t_{1/2} = 2.096 \text{ d from river, 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002)}$.

Groundwater:

Sediment: uptake clearance from sediment was $(0.0021 \pm 0.001) \text{ g of dry sediment-g}^{-1} \text{ of organism-h}^{-1} \text{ for amphipod, } P. hoyi \text{ in Lake Michigan sediments at 4°C (Landrum 1989);}$
$k(\text{exptl}) < 0.9 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 2.7–6.3, with } t_{1/2} > 7 \text{ h at pH 7 and 23 ± 2°C (Yao & Haag 1991).}$
$t_{1/2} = 165000 \text{ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Soil: $t_{1/2} = 165000 \text{ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Biota: half-life in rainbow trout, > 1000 d and its muscle, 77 d (Niimi & Oliver 1983);
$t_{1/2} = 170 \text{ d in worms at 8°C (Oliver 1987c); } t_{1/2} = 175 \text{ d in guppy (Bruggeman et al. 1984); } t_{1/2} = 45.6 \text{ d in Pontoporeia hoyi (Evans & Landrum 1989); elimination } t_{1/2} = 15.9 \text{ d from earthworm (Belfroid et al. 1995)}$.

Depuration $t_{1/2} = 69–224 \text{ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998); thetheoretical } t_{1/2} = 25.7 \text{ d to reach 90% steady-state tissue concn (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999); } t_{1/2} = 5.1 \text{ h in blood plasma (ring doves, Drouillard & Norstrom 2000); elimination } t_{1/2} = 18 \text{ d in earthworm given contaminated food (Wågman et al. 2001).}$

depuration $t_{1/2} = 177 \text{ d for high-dose treatment, } t_{1/2} = 219 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)}$
depuration $t_{1/2} = 46.2 \text{ d (juvenile carp in 100-d experiment Stapleton et al. 2004)}$
<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Doucette &amp; Andren 1988</strong></td>
<td><strong>Bamford et al. 2000</strong></td>
<td><strong>Harner &amp; Bidleman 1996</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas stripping-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/(g·m⁻³)</td>
<td>t/°C</td>
</tr>
<tr>
<td>4</td>
<td>0.00462</td>
<td>4</td>
</tr>
<tr>
<td>25</td>
<td>0.00845</td>
<td>11</td>
</tr>
<tr>
<td>40</td>
<td>0.0128</td>
<td>18</td>
</tr>
<tr>
<td>25</td>
<td>52.8</td>
<td>25</td>
</tr>
<tr>
<td>31</td>
<td>91.2</td>
<td>30</td>
</tr>
</tbody>
</table>

S/(mol/L) = A·exp[B·(t/°C)]
A = 1.15 × 10⁻⁸
B = 0.028

ΔH_{sol}/(kJ·mol⁻¹) = 20.3
for 4–40°C

enthalpy, entropy change:
ΔH/(kJ·mol⁻¹) = 66.1 ± 5.4
ΔS/(J·mol⁻¹·K⁻¹) = 190 ± 18

**FIGURE 7.1.1.153.1** Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',4,4',5,5'-hexachlorobiphenyl (PCB-153).
7.1.1.154 2,2’,4,4’,5,6’-Hexachlorobiphenyl (PCB-154)

Common Name: 2,2’,4,4’,5,6’-Hexachlorobiphenyl
Synonym: PCB-154, 2,2’,4,4’,5,6’-hexachloro-1,1’-biphenyl
Chemical Name: 2,2’,4,4’,5,6’-hexachlorobiphenyl
CAS Registry No: 60145-22-4
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
- oil (Erickson 1986)
- 117 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
- 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
- 0.0106 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00173, 0.00137, 0.00293, 0.00213 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 1.71 × 10⁻³ (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 1.86 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985b)
- 0.00182 (supercooled liquid P_{L}, GC-RI correlation, Fischer et al. 1992)
log (P_{L}/Pa) = -4681/(T/K) + 12.94 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
- 58.46 (calculated-P/C, Burkhard 1984)
- 48.84 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
- 38.7 (calculated-QSPR, Dunnivant et al. 1992)
- 17.34, 29.16, 47.85, 76.7 ± 2.2, 113.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 15.155 – 5556.89/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[–(46.2/kJ·mol⁻¹)/RT] + (0.126/kJ·mol⁻¹·K⁻¹)/R]; where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
- 75.4 (exptl. data, Bamford et al. 2002)
ln K_{AW} = -ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 46 ± 5 kJ/mol, ΔS_{f} = 0.13 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
- 6.87 (calculated-TSA, Burkhard 1984)
- 6.67, 6.81, 6.47, 6.64 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.76 (calculated-TSA, Hawker & Connell 1988a)
- 7.05, 7.03; 6.48, 6.43 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.65 (recommended, Sangster 1993)
6.89 (recommended, Hansch et al. 1995)
6.6326 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{OA}$:
9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
6.66 (suspended particulate matter, Burkhard 1984)
5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16–0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.155 2,2′,4,4′,6,6′-Hexachlorobiphenyl (PCB-155)

Common Name: 2,2′,4,4′,6,6′-Hexachlorobiphenyl
Synonym: PCB-155, 2,2′,4,4′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6,6′-hexachlorobiphenyl
CAS Registry No: 33979-03-2
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
  112.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.3482
Molar Volume (cm³/mol):
  310.0 (calculated-Le Bas method at normal boiling point)
  237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHₘₒₜ (kJ/mol):
  17.5 (differential scanning calorimetry, Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
  20.30 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔSₘₒₜ (J/mol K):
  45.19 (Miller et al. 1984)
  45.25, 66.9 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSₘₒₜ = 56 J/mol K), F:
  0.139 (mp at 112.5°C)
  0.131 (Mackay et al. 1980; Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section):
  0.00090 (generator column-GC/ECD, Weil et al. 1974)
  0.00041 (generator column-GC/ECD, Miller et al. 1984,1985)
  0.0000528 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
  2.50 × 10⁻³, 1.34 × 10⁻³, 6.27 × 10⁻³, 2.68 × 10⁻³ (RP-HPLC-k correlation, different stationary and mobile phases,
  Brodsky & Ballshmoter 1988)
  0.0023 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
  0.00109 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
  0.00033 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
  0.00284 (shake flask-GC/ECD, Li & Andre 1994)
  0.0028* ± 0.00013 (generator column-GC/ECD, Shiu et al. 1997)
  1.89 × 10⁻¹, 0.0050 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  ln x = –8.9206 – 4112.07/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
  0.0142, 0.0138 (supercooled liquid Sₜ ; derivation of literature-derived value LDV, final-adjusted value FAV, Li
  et al. 2003)
  log [Sₜ/(mol m⁻³)] = –861/(T/K) – 1.52 (supercooled liquid, linear regression of literature data, Li et al. 2003)
  log [Sₜ/(mol m⁻³)] = –1268/(T/K) – 0.16 (supercooled liquid, final adjusted eq., Li et al. 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  0.0016 (GC-RT, Westcott et al. 1981)
  0.0122 (Pₚ calculated from Pₛ using fugacity ratio F, Westcott et al. 1981)
  0.0017 (gas saturation, Westcott & Bidleman 1981)
  0.00443 (supercooled liquid Pₚ, Burkhard 1984)
3.57 × 10⁻⁴, 6.41 × 10⁻⁴, 8.04 × 10⁻¹ (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985a)
0.00443 (supercooled liquid $P_L$, GC-RI correlation, Burkhard et al. 1985b)
0.00159, 0.012 (selected $P_S$, $P_L$, Shiu & Mackay 1986)
4.76 × 10⁻⁴ (calculated-$S \times HLC$, Dunnivant & Elzerman 1988)
3.54 × 10⁻⁴ (supercooled liquid $P_L$, calculated-mp, Dunnivant & Elzerman 1988)

$\log (P_L/P_a) = -\frac{3403}{T/K} + 12.02$ (supercooled liquid $P_L$, GC-RT correlation, Falconer & Bidleman 1994)
$3.25 \times 10^{-16}$ (gas saturation-GC/ECD, measured range –10 to 30°C, Wania et al. 1994)
$\log (P_L/P_a) = 14.84 - 5399/(T/K)$; temp range –10 to 30°C (gas saturation-GC, Wania et al. 1994)
$2.188 \times 10^{-3}$ (20°C, supercooled liquid $P_L$ from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
11.65 (gas stripping-GC, Coates 1984)
157.0 (calculated-P/C, Burkhard et al. 1985b)
12.46 (calculated, Coates & Elzerman 1986)
817.9 (calculated-P/C, Shiu & Mackay 1986)
76.5 (gas stripping-GC, Dunnivant et al. 1988, Dunnivant & Elzerman 1988)
60.8 (calculated-QSAR-MCI $\chi$, Sabljic & Güsten 1989)
85.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

Octanol/Water Partition Coefficient, log $K_{OW}$:
6.70 (shake flask-GC, Chiou et al. 1977)
6.34 (shake flask-GC, Karickhoff et al. 1979)
6.37 (HPLC-$k'_{correlation}$, McDuffie 1981)
7.12 (RP-TLC-$k'_{correlation}$, Bruggeman et al. 1982)
6.88 (calculated-TSA, Burkhard 1984)
7.55 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.39 (HPLC-RT/MS correlation, Burkhard et al. 1985c)
6.01 (HPLC-$k'_{correlation}$, Tomlinson & Hafkenscheid 1986)
7.24 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
6.54, 6.81, 6.24, 6.57 (RP-HPLC-RI correlations, Brodsky & Ballschmiter 1988)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.287 ± 0.065 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.08, 7.03; 6.24, 6.22 (multi-column HPLC-$k'_{correlation}$; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (HPLC-$k'_{correlation}$, Noegrohati & Hammers 1992)
7.24 (shake flask-GC/ECD, Li & Doucette 1993)
6.54 (recommended, Sangster 1993)
7.29 (recommended, Hansch et al. 1995)
7.36, 7.19 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
8.99* (generator column-GC/ECD; measured range –10 to +20°C; Harner & Mackay 1995)
$\log K_{OA} = -2.20 + 3954/(T/K)$; (temp range –10 to +20°C, generator column-GC, Harner & Mackay 1995)
Polychlorinated Biphenyls (PCBs)

log $K_{OA} = -2.21 + 3954/(T/K)$; temp range -10 to +20°C (generator column-GC, Harner & Bidleman 1996)
10.19, 9.13; 9.16 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.24 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.89, 9.14 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log $K_{OA} = 4357/(T/K) - 5.47$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:
1.02 (poultry, Garten & Trabalka 1983)
2.79–3.68 highest value 3.68, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7-d to 96-d laboratory study, Oliver & Niimi 1985)
> 4.94; 3.68 (rainbow trout, laboratory data: kinetic BCF ($k_1/k_2$), steady-state BCF ($C_p/C_w$), Oliver & Niimi 1985)
4.53 (worms, Oliver 1987c)
3.68 (fish, Isnard & Lambert 1988)
5.99, 7.29 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
6.08 (natural sediment, sorption isotherm by batch equilibrium technique-GC, Karickhoff et al. 1979)
5.95, 7.28, 5.95(calculated-$K_{OC}$, calculated-$C_1$, calculated-$C_2$, Karickhoff 1981)
6.68 (suspended particulate matter, calculated-$K_{OC}$, Burkhard 1984)
4.905 (calculated-MCI $\chi$, marine humic substances with 5 mg/L of DOC, reported as association coefficient log $K_w$, Sabljic et al. 1989)
6.08; 6.17 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_h$:

Volatilization:

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$, or as indicated, *data at other temperatures see reference:
$k_{OH}$(calc) = (0.16 – 0.5) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 8.6–29.5 \text{ h}^{-1}$ in pond-sediment system, $k_1 = 22.9–14.6 \text{ h}^{-1}$ in river-water system, $k_1 = 29.6–39.8 \text{ h}^{-1}$ in river-send system, $k_1 = 26.7–47.0 \text{ h}^{-1}$ in sand-sediment system ($Chironomus tentans$ larvae, Muir et al. 1983)
$k_2 = 0.0029 \text{ h}^{-1}$ with $t_{h_2} = 241 \text{ h}$ in pond-sediment system, $k_2 = 0.0059 \text{ h}^{-1}$ with $t_{h_2} = 117 \text{ h}$ in river-water system, $k_2 = 0.0034 \text{ h}^{-1}$ with $t_{h_2} = 203 \text{ h}$ in river-send system, $k_2 = 0.0030 \text{ h}^{-1}$ with $t_{h_2} = 230 \text{ h}$ in sand-sediment system ($Chironomus tentans$ larvae, Muir et al. 1983)
$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 60 \text{ d}^{-1}$; $k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985; Thomann 1989)
log 1/$k_2 = 3.1$, 3.6 h (fish, quoted, calculated-$K_{OC}$, Hawker & Connell 1988b)
1/($k_2$) = 141 d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:
1882 Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Biota: $t_{1/2} = 117–241$ h in sediment-water systems (*Chironomus tentans* larvae, Muir et al. 1983)
$t_{1/2} > 1000$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2} = 77$ d in its muscle (Niimi & Oliver 1983).

### TABLE 7.1.1.155.1
Reported aqueous solubilities and octanol-air partition coefficients log of 2,2',4,4',6,6' -hexachlorobiphenyl (PCB-155) at various temperatures and the reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Shiu et al. 1997</strong></td>
<td><strong>Wania et al. 1994</strong></td>
<td><strong>Harner &amp; Mackay 1995</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>$1.0 \times 10^{-3}$</td>
<td>-10</td>
</tr>
<tr>
<td>15</td>
<td>$1.70 \times 10^{-3}$</td>
<td>0</td>
</tr>
<tr>
<td>25</td>
<td>$2.80 \times 10^{-3}$</td>
<td>10</td>
</tr>
<tr>
<td>35</td>
<td>$4.30 \times 10^{-3}$</td>
<td>20</td>
</tr>
<tr>
<td>45</td>
<td>$6.40 \times 10^{-3}$</td>
<td>30</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}/(kJ \text{ mol}^{-1}) = 34.2$ 
for 5–45°C

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 63.9$

$\Delta H_{subl}/(kJ \text{ mol}^{-1}) = 103.4$

$\log (P/Pa) = A - B/(T/K)$

$A = 14.84$

$B = 5399$

$log K_{OA} = A + B/RT$

$A = -2.2$

$B = 3337.4$

### FIGURE 7.1.1.155.1
Logarithm of vapor pressure and $K_{OA}$ versus reciprocal temperature for 2,2',4,4',6,6' -hexachlorobiphenyl (PCB-155).
7.1.1.156 2,3,3',4,4',5-Hexachlorobiphenyl (PCB-156)

Common Name: 2,3,3',4,4',5-Hexachlorobiphenyl
Synonym: PCB-156, 2,3,3',4,4',5-hexachloro-1,1'-biphenyl
Chemical Name: 2,3,3',4,4',5-hexachlorobiphenyl
CAS Registry No: 38380-08-4
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
127 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F: 0.100 (mp at 127°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0033 (20°C, supercooled liquid S_{L}, Murphy et al. 1987)
0.00361, 0.00244, 0.00112, 0.00102 (RP-HPLC-k correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
0.000397 (generator column-GC/ECD, Hong & Qiao 1995)
0.0011 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000513, 0.000711, 0.00110, 0.00153 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000215 (supercooled liquid P_{L}, GC-RT correlation, Bidleman 1984)
7.34 × 10⁻⁴ (supercooled liquid P_{L}, GC-RT correlation, Burkhard et al. 1985a)
0.000809 (GC-RI correlation, Burkhard et al. 1985b)
0.00021, 0.00016 (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.26 × 10⁻⁴, 1.62 × 10⁻⁴ (supercooled liquid P_{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = -4949/(T/K) + 12.94 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
88.14 (concn ratio-GC, Murphy & Mullin 1983)
17.53 (calculated-P/C, Burkhard et al. 1985)
2.23 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
8.97 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
3.72 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
37.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = -ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 112 ± 10 kJ/mol, ΔS_{fus} = 0.34 ± 0.03 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

© 2006 by Taylor & Francis Group, LLC
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 7.13, 7.26, 7.84, 7.53 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 7.14, 7.12, 7.16, 7.13 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.70 (generator column-GC, Larsen et al. 1992)
- 7.11 (recommended, Sangster 1993)
- 7.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 12.07, 10.87; 10.87 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
- 5.88, 7.18 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.51 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.40 (as log $K_a$, association coefficient with marine humic substance, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH(calc)} = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_2 = 0.024$ d$^{-1}$ with an elimination $t_\frac{1}{2} = 29$ d (earthworm, Belfroid et al. 1995)
- $k_2 = 0.004$ d$^{-1}$ with $t_\frac{1}{2} = 163$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_\frac{1}{2} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: clearance $t_\frac{1}{2} = 50–100$ d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for hexachlorobiphenyls: $t_\frac{1}{2} = 87$ to $> 850$ d for trout, $t_\frac{1}{2} = 77–91$ d for trout muscle; $t_\frac{1}{2} > 200$ d for carp; $t_\frac{1}{2} = 75–175$ d for guppy (Niimi 1987);

elimination $t_\frac{1}{2} = 29$ d from earthworm (Belfroid et al. 1995)

depuration $t_\frac{1}{2} = 163$ d for high-dose treatment, $t_\frac{1}{2} = 182$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
### 7.1.1.157 2,3',4,4',5'-Hexachlorobiphenyl (PCB-157)

![Chemical Structure](image)

**Common Name:** 2,3',4,4',5'-Hexachlorobiphenyl  
**Synonym:** PCB-157, 2,3',4,4',5'-hexachloro-1,1'-biphenyl  
**Chemical Name:** 2,3',4,4',5'-hexachlorobiphenyl  
**CAS Registry No:** 69782-90-7  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{4}Cl\textsubscript{6}  
**Molecular Weight:** 360.878

<table>
<thead>
<tr>
<th>Physical Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>141 (estimated-molecular properties, Abramowitz &amp; Yalkowsky 1990)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm\textsuperscript{3})</td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm\textsuperscript{3}/mol)</td>
<td>310.0 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, $\Delta H\text{fus}$ (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, $\Delta S\text{fus}$ (J/mol K)</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming $\Delta S\text{fus} = 56$ J/mol K), $F$</td>
<td></td>
</tr>
</tbody>
</table>

**Water Solubility** (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations):

- 0.0152 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
- 0.000119 (generator column-GC/ECD, Hong & Qiao 1995)
- 0.000296 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
- 0.000084, 0.000139, 0.000296, 0.000540 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

**Vapor Pressure** (Pa at 25°C and reported temperature dependence equations):

- 1.39 × 10\textsuperscript{-4} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 8.09 × 10\textsuperscript{-4} (GC-RI correlation, Burkhard et al. 1985b)
- 2.02 × 10\textsuperscript{-4}, 1.27 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}, GC-RT correlation; different stationary phases, Foreman & Bidleman 1985)
- 1.17 × 10\textsuperscript{-4}, 1.58 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}, GC-RI correlation, different stationary phases, Fischer et al. 1992)
- log (P\textsubscript{L}/Pa) = –4994/(T/K) + 13.05 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

**Henry’s Law Constant** (Pa·m\textsuperscript{3}/mol at 25°C):

- 3.30 (calculated-P/C, Burkhard et al. 1985a)
- 58.76 (concn ratio-GC, Murphy & Mullin 1983)
- 6.69 (calculated-QSPR-MCI $\chi$, Sabljic & Güsten 1989)
- 8.56 (calculated-QSPR, Dunnivant et al. 1992)
- 1.50 (calculated-QSPR, Achman et al. 1993)
- 2.27 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
- 31.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_{fus}/RT + \Delta S_{fus}/R; \text{ R is the ideal gas constant, } \Delta H_{H} = 129 \pm 10 \text{ kJ/mol, } \Delta S_{H} = 0.40 \pm 0.03 \text{ kJ/mol·K} \]

- 31.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)—see Comment by Goss et al. 2004

**Octanol/Water Partition Coefficient, log $K_{OW}$**:

- 7.18 (calculated-TSA, Hawker & Connell 1988a)
- 7.26, 7.14; 7.19, 7.04 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 7.20 (quoted average values of Risby et al. 1990: GC-RV and HPLC-k’ correlations, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

- 12.28, 11.07, 10.76 (0, 20°C, multi-column GC-κ' correlation; calculated at 20°C, Zhang et al. 1999)
- 10.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{B}$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.51 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.40 (as log $K_{h}$, association coefficient with marine humic substance, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for hexachlorobiphenyls, and the tropospheric lifetime } \tau(calc) = 29–60 \text{ d} \text{ at room temp. (Kwok et al. 1995)}$$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: clearance $t_{1/2} = 50–100$ d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984); reported biological half-lives for hexachlorobiphenyls: $t_{1/2} =$ 87 to > 850 d for trout, $t_{1/2} =$ 77–91 d for trout muscle; $t_{1/2} > 200$ d for carp; $t_{1/2} =$ 75–175 d for guppy (Niimi 1987)
7.1.1.158  2,3,3',4,4',6-Hexachlorobiphenyl (PCB-158)

Common Name: 2,3,3',4,4',6-Hexachlorobiphenyl
Synonym: PCB-158, 2,3,3',4,4',6-hexachloro-1,1'-biphenyl
Chemical Name: 2,3,3',4,4',6-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: C_{12}H_4Cl_6
Molecular Weight: 360.878
Melting Point (°C):
  107  (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  310.0  (calculated-Le Bas method at normal boiling point)
  237.4  (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.157 (mp at 107°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  0.0159  (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  0.00807 (20°C, supercooled liquid, Murphy et al. 1987)
  0.00120 (RP-HPLC-k correlation, Brodsky & Ballschmieder 1988)
  0.00114 (TSA and mp, Abramowitz & Yalkowsky 1990)
  0.00185 (calculated-group contribution method, Kühne et al. 1995)
  0.00147, 0.00396 (molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  9.26 \times 10^{-4}  (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  1.02 \times 10^{-3}  (GC-R1 correlation, Burkhard et al. 1985b)
  6.19 \times 10^{-4}, 4.486 \times 10^{-4}  (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  9.73 \times 10^{-5}  (20°C, supercooled liquid, Murphy et al. 1987)
  3.09 \times 10^{-4}, 4.57 \times 10^{-4}  (supercooled liquid P_L, GC-R1 correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4816/(T/K) + 12.94  (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  20.97  (calculated-P/C, Burkhard 1984)
  4.37  (20°C, calculated-P/C, Murphy et al. 1987)
  21.89  (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
  2.86  (calculated-QSPR, Achman et al. 1993)
  16.74  (calculated-QSPR, Dunnivant et al. 1992)
  9.64  (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
  49.9  (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –\Delta H_{fus}/RT + \Delta S_{fus}/R;  R is the ideal gas constant, \Delta H_{fus} = 80 ± 7 kJ/mol, \Delta S_{fus} = 0.24 ± 0.02 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 6.69 (calculated-TSA, Burkhard 1984)
- 6.78 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
- 7.02 (calculated-TSA, Hawker & Connell 1988a)
- 7.10, 6.87, 6.84, 6.82 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.78 (recommended, Sangster 1993)
- 7.25 (recommended, Hansch et al. 1995)
- 6.874 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.
- 9.51; 9.12 (generator column-GC.; $K_{OW}/K_{AW}$, Kömp & McLachlan 1997a)
- $K_{OA} = -5.17 + 4380/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)
- 10.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_{bi}$:

Sorption Partition Coefficient, log $K_{oc}$:
- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_1/2$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 0.006$ d$^{-1}$ with $t_{1/2} = 124$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.003$ d$^{-1}$ with $t_{1/2} = 241$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 124$ d for high-dose treatment, $t_{1/2} = 241$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.159 2,3,3’,4,5,5’-Hexachlorobiphenyl (PCB-159)

Common Name: 2,3,3’,4,5,5’-Hexachlorobiphenyl
Synonym: PCB-159, 2,3,3’,4,5,5’-hexachloro-1,1’-biphenyl
Chemical Name: 2,3,3’,4,5,5’-hexachlorobiphenyl
CAS Registry No: 39635-35-3
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
   116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   0.0135 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
   5.72 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
   1.084 × 10⁻³ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
   0.00119 (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   29.08 (calculated-P/C, Burkhard 1984)
   31.41 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
   2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)
   15.77 (calculated-QSPR, Dunnivant et al. 1992)
   35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
   ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 116 ± 12 kJ/mol, ΔS_{f} = 0.35 ± 0.04 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
   6.76 (calculated-TSA, Burkhard 1984)
   7.24 (calculated-TSA, Hawker & Connell 1988a)
   7.09, 7.24; 7.02, 7.00 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
   7.17, 7.01 (quoted average values of Risby et al. 1990, Sangster 1993)
   7.43 (recommended, Hansch et al. 1995)
   7.2038 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
   10.37 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.56 (suspended particulate matter, Burkhard 1984)
- 5.381 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference: $k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \text{ d at room temp.}$ (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
7.1.1.160 2,3,3′,4,5,6-Hexachlorobiphenyl (PCB-160)

Common Name: 2,3,3′,4,5,6-Hexachlorobiphenyl
Synonym: PCB-160, 2,3,3′,4,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,6-hexachlorobiphenyl
CAS Registry No: 41411-62-5
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
99  (Burkhard et al. 1985b)
97–100  (Erickson 1986)
Boiling Point (°C):
Density (g/cm³):
310.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.188  (mp at 99°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.0191  (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00158  (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C):
1.33 × 10⁻³  (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00027  (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
25.13  (calculated-P/C, Burkhard 1984)
25.74  (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.027  (wetted wall column-GC/ECD, Brunner et al. 1990)
21.66  (calculated-QSPR, Dunnivant et al. 1992)
49.5  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_fus/RT + ΔS_fus/R; R is the ideal gas constant, ΔH_fus = 79 ± 18 kJ/mol, ΔS_fus = 0.23 ± 0.06 kJ/mol-K
Octanol/Water Partition Coefficient, log K_{OW}:
6.62  (calculated-TSA, Burkhard 1984)
6.93  (calculated-TSA, Hawker & Connell 1988a)
6.88, 6.79; 6.89, 6.87  (multi-column HPLC-k⁺ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.84, 6.88  (quoted average values of Risby et al. 1990, Sangster 1993)
7.30  (recommended, Hansch et al. 1995)
6.9006  (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
10.05  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, $\log K_{OC}$:
- 6.42 (suspended particulate matter, Burkhard 1984)
- 5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O_3$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.161 2,3′,4,5′,6-Hexachlorobiphenyl (PCB-161)

Common Name: 2,3′,4,5′,6-Hexachlorobiphenyl  
Synonym: PCB-161, 2,3′,4,5′,6-hexachloro-1,1′-biphenyl  
Chemical Name: 2,3′,4,5′,6-hexachlorobiphenyl  
CAS Registry No: 74472-43-8  
Molecular Formula: C_{12}H_{4}Cl_{6}  
Molecular Weight: 360.878  
Melting Point (°C):  
84.0  
(estimated, Abramowitz & Yalkowsky 1990)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
310.0  
(calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):  
Entropy of Fusion, ∆S_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
0.0141  
(Sₗ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00181  
(calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
Vapor Pressure (Pa at 25°C):  
1.37 × 10⁻³  
(Pₗ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
0.00150  
(GC-RI correlation, Burkhard et al. 1985b)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
34.96  
(calculated-P/C, Burkhard 1984)  
51.27  
(calculated-QSPR-MCI χ, Sabljic & Güsten 1989)  
28.89  
(calculated-QSPR, Dunnivant et al. 1992)  
49.5  
(predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
ln K_{OW} = –∆H_{f}_/RT + ∆S_{f}/R; R is the ideal gas constant, ∆H_{f} = 79 ± 18 kJ/mol, ∆S_{f} = 0.23 ± 0.06 kJ/mol-K  
(Bamford et al. 2002)—see Comment by Goss et al. 2004  
Octanol/Water Partition Coefficient, log K_{OW}:  
6.76  
(calculated-TSA, Burkhard 1984)  
7.08  
(calculated-TSA, Hawker & Connell 1988a)  
7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)  
7.05, 6.68  
(quoted average values of Risby et al. 1990, Sangster 1993)  
7.10  
(recommended, Hansch et al. 1995)  
7.0318  
(calculated-molecular properties MNDO-AM1 method, Makino 1998)  
Octanol/Air Partition Coefficient, log K_{OA}:  
10.33  
(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)  
Bioconcentration Factor, log BCF or log K_{H}:
Sorption Partition Coefficient, log $K_{OC}$:

- 6.56 (suspended particulate matter, Burkhard 1984)
- 5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$$k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60 \text{ d at room temp.}$ (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.162 2,3′,4′,5,5′-Hexachlorobiphenyl (PCB-162)

Common Name: 2,3′,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-162, 2,3′,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3′,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 39635-34-2
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878

Melting Point (°C):
84.0 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0141 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.37 × 10⁻³ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry’s Law Constant (Pa-m³/mol at 25°C):
34.96 (calculated-P/C, Burkhard 1984)
51.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
28.89 (calculated-QSPR, Dunnivant et al. 1992)
35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\[
\ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; R \text{ is the ideal gas constant, } \Delta H_{f} = 116 \pm 12 \text{ kJ/mol, } \Delta S_{f} = 0.35 \pm 0.04 \text{ kJ/mol K}
\]
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.08 (calculated-TSA, Hawker & Connell 1988a)
7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)
7.10 (recommended, Hansch et al. 1995)
7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, $\log K_{OC}$:

- 6.56 (suspended particulate matter, Burkhard 1984)
- 5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  $k_{OH}(calc) = (0.16 – 0.5)\times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
7.1.1.163 2,3,3',4',5,6-Hexachlorobiphenyl (PCB-163)

![Chemical Structure of 2,3,3',4',5,6-Hexachlorobiphenyl (PCB-163)]

Common Name: 2,3,3',4',5,6-Hexachlorobiphenyl
Synonym: PCB-163, 2,3,3',4',5,6-hexachloro-1,1'-biphenyl
Chemical Name: 2,3,3',4',5,6-hexachlorobiphenyl
CAS Registry No: 74472-44-9
Molecular Formula: C_{12}H_4Cl_{16}
Molecular Weight: 360.878

Melting Point (°C):
- 88.2 (Shiu & Mackay 1986)
- 122 (Ran et al. 2002)

Boiling Point (°C):

Density (g/cm³):
- 310.0 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm³/mol):

Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):

Fugacity Ratio at 25°C, F:
- 0.237 (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.00531 (generator column-HPLC/UV, Huang 1983)
- 0.0053 (generator column-HPLC/UV, Billington et al. 1988)
- 0.0012 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- $8.67 \times 10^{-4}$ (Pc supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- $9.54 \times 10^{-4}$ (GC-RI correlation, Burkhard et al. 1985b)
- $6.01 \times 10^{-4}$, $4.92 \times 10^{-4}$ (supercooled liquid Pc, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- $3.31 \times 10^{-4}$, $5.25 \times 10^{-4}$ (supercooled liquid Pc, GC-RI correlation, different stationary phases, Fischer et al. 1992)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 18.54 (calculated-P/C, Burkhard 1984)
- 11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
- 1.52 (wetted wall column-GC/ECD, Brunner et al. 1990)
- 12.73 (calculated-QSPR, Dunnivant et al. 1992)

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
- 6.78 (calculated-P/C, Burkhard 1984)
- 7.08; 6.99; 6.84, 6.79 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.39 (generator column-GC, average, Larsen et al. 1992)
- 6.78 (recommended, Sangster 1993)
- 7.25 (recommended, Hansch et al. 1995)

Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ = $81 \pm 7$ kJ/mol, $\Delta S_{\text{ fus}} = 0.24 \pm 0.02$ kJ/mol·K

From 11°C exptl. data and compensation point, Bamford et al. 2002
$\ln K_{\text{AW}} = -\Delta H_{\text{ fus}}/RT + \Delta S_{\text{ fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{ fus}} = 81 \pm 7$ kJ/mol, $\Delta S_{\text{ fus}} = 0.24 \pm 0.02$ kJ/mol·K

Log $K_{\text{ow}}$—see Comment by Goss et al. 2004

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 11.26, 10.16 (0, 20°C, multi-column GC-k correlation, Zhang et al. 1999)
- 9.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.47 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29$–$60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 170$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d$^{-1}$ with $t_{1/2} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 170$ d for high-dose treatment, $t_{1/2} = 198$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.164 2,3,3',4',5',6-Hexachlorobiphenyl (PCB-164)

![Chemical Structure]

Common Name: 2,3,3',4',5',6-Hexachlorobiphenyl
Synonym: PCB-164, 2,3,3',4',5',6-hexachloro-1,1'-biphenyl
Chemical Name: 2,3,3',4',5',6-hexachlorobiphenyl
CAS Registry No: 74472-45-0
Molecular Formula: C_{12}H_{4}Cl_{6}
Molecular Weight: 360.878
Melting Point (°C):
96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0161 (S_{ L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00194 (RP-HPLC-k' correlation, Brodsky & Ballischeimer 1988)
0.00144 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
4.478 × 10⁻⁴ (P_{ L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.97 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
10.04 (calculated-P/C, Burkhard 1984)
19.96 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
17.41 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group andortho-Cl, Bamford et al. 2002)
ln K_{ AW} = −ΔH_{ H}/RT + ΔS_{ H}/R; R is the ideal gas constant, ΔH_{ H} = 79 ± 18 kJ/mol, ΔS_{ H} = 0.23 ± 0.03 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ OW}:
6.69 (calculated-TSA, Burkhard 1984)
6.63 (RP-HPLC-k’ correlation, Brodsky & Ballischeimer 1988)
7.02 (calculated-TSA, Hawker & Connell 1988a)
7.22, 7.32; 6.79, 6.73 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.63 (recommended, Sangster 1993)
7.20 (recommended, Hansch et al. 1995)
6.6712 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{ OA}:
10.35 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference: $k_{OH(calc)} = (0.16 – 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 29–60$ d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
Common Name: 2,3',5,5',6-Hexachlorobiphenyl
Synonym: PCB-165, 2,3',5,5',6-hexachloro-1,1'-biphenyl
Chemical Name: 2,3',5,5',6-hexachlorobiphenyl
CAS Registry No: 74472-46-1
Molecular Formula: C_{12}H_4Cl_6
Molecular Weight: 360.878
Melting Point (°C): 101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³): 310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0150 (S_1 supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
1.292 × 10⁻³ (P_1 supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00140 (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
30.9 (calculated-P/C, Burkhard 1984)
45.19 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.94 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.91 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −∆H/R + ∆S/R; R is the ideal gas constant, ∆H = 79 ± 18 kJ/mol, ∆S = 0.23 ± 0.06 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
6.57, 7.37 (RP-HPLC-k’ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.72 (calculated-TSA, Burkhard 1984)
7.05 (calculated-TSA, Hawker & Connell 1988a)
7.17, 6.90; 6.70, 6.65 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.37, 6.68, 7.04 (quoted literature values, Sangster 1993)
7.37 (recommended, Hansch et al. 1995)
7.0191 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA}:
9.88 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log $K_{OC}$:
- 6.52 (suspended particulate matter, Burkhard 1984)
- 5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29$–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
Polychlorinated Biphenyls (PCBs)

7.1.1.166 2,3,4,4',5,6-Hexachlorobiphenyl (PCB-166)

Common Name: 2,3,4,4',5,6-Hexachlorobiphenyl
Synonym: PCB-166, 2,3,4,4',5,6-hexachloro-1,1'-biphenyl
Chemical Name: 2,3,4,4',5,6-hexachlorobiphenyl
CAS Registry No: 41411-63-6
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878

Melting Point (°C):
- 163.0 (Burkhard et al. 1985b)
- 160–165 (Erickson 1986)
- 145 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
- 310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH₉₉ (kJ/mol):

Entropy of Fusion, ΔS₉₉ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS₉₉ = 56 J/mol K), F: 0.0443 (mp at 163°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0189 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 7.20 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
- 2.46 × 10⁻⁴ (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
- 1.175 × 10⁻³ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 22.49 (calculated-P/C, Burkhard 1984)
- 17.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
- 18.65 (calculated-QSPR, Dunnivant et al. 1992)
- 49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln Kₐw = −ΔH₉₉/RT + ΔS₉₉/R; R is the ideal gas constant, ΔH₉₉ = 79 ± 18 kJ/mol, ΔS₉₉ = 0.23 ± 0.06 kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K₀ₗₗ:
- 6.62 (calculated-TSA, Burkhard 1984)
- 6.93 (calculated-TSA, Hawker & Connell 1988a)
- 7.13, 7.18; 6.90, 6.83 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 7.17, 6.87 (quoted average values of Risby et al. 1990, Sangster 1993)
- 7.31 (recommended, Hansch et al. 1995)
- 6.8501 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K₀ₐₐ:
- 10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_OC:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.42</td>
<td>(suspended particulate matter, Burkhard 1984)</td>
</tr>
<tr>
<td>5.259</td>
<td>(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_a, calculated-molecular connectivity indices, Sabljic et al. 1989)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k, and Half-Lives, t½:

- **Volatilization**:
- **Photolysis**:
- **Oxidation**: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O3} with O₃ or as indicated, *data at other temperatures see reference: k_{OH}(calc) = (0.16 – 0.5) × 10^{-12} cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
- **Hydrolysis**:
- **Biodegradation**:
- **Biotransformation**:
- **Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):**

Half-Lives in the Environment:

- **Air**: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- **Surface water**:
- **Ground water**:
- **Sediment**:
- **Soil**:
- **Biota**:
7.1.1.167 2,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-167)

![Chemical Structure](image)

Common Name: 2,3′,4,4′,5,5′-Hexachlorobiphenyl

Synonym: PCB-167, 2,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl

Chemical Name: 2,3′,4,4′,5,5′-hexachlorobiphenyl

CAS Registry No: 52663-72-6

Molecular Formula: C_{12}H_4Cl_6

Molecular Weight: 360.878

Melting Point (°C): 135 (calculated-molecular properties, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0128 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00223 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)

0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.000531 (generator column-GC/ECD, Hong & Qiao 1995)

0.000107 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004

0.000442, 0.000682, 0.00107, 0.00161 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.88 × 10⁻⁴ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

2.12 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)

2.80 × 10⁻⁴, 2.39 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.34 × 10⁻⁴ (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)

log (P₁/Pa) = –4994/(T/K) + 13.20 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m⁻³/mol at 25°C):

5.33 (calculated-P/C, Burkhard et al. 1985a)

12.46 (calculated-QSPr-MClₓ, Sabljic & Güsten 1989)

20.55 (calculated-QSPr, Dunnivant et al. 1992)

4.47 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

39.28 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 106 ± 8 kJ/mol, ΔS_{f} = 0.32 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{o/w}:

7.29 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)

7.24, 7.30; 7.00, 7.03 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.29 (recommended, Sangster 1993)

7.50 (recommended, Hansch et al. 1995)

6.82 (generator column-GC/ECD, Yeh & Hong 2002)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or indicated:

- 12.07, 10.77; 10.76 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.59 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

- 5.97, 7.27 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.58 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.381 (as log $K_h$, association coefficient with marine humic substance, calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Vaporization:**

**Photolysis:**

**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH}$(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 29–60 d at room temp. (Kwok et al. 1995)

**Hydrolysis:**

**Biodegradation:**

**Bioregulation:**

**Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**

- $k_2 = 0.0263$ d$^{-1}$ with an elimination $t_{1/2} = 26$ d (earthworm, Belfroid et al. 1995)
- $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 134$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005$ d$^{-1}$ with $t_{1/2} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

**Air:** the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

**Surface water:** photodegradation $t_{1/2} = 38$ min when irradiated in a TiO$_2$ semiconductor aqueous suspension with a 1.5-kW Xenon lamp (De Felip et al. 1996)

**Ground water:**

**Sediment:**

**Soil:**

**Biota:** clearance $t_{1/2} = 50–100$ d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for hexachlorobiphenyls: $t_{1/2} = 87$ to $> 850$ d for trout, $t_{1/2} = 77–91$ d for trout muscle; $t_{1/2} > 200$ d for carp; $t_{1/2} = 75–175$ d for guppy (Niimi 1987);

elimination $t_{1/2} = 26.4$ d from earthworm (Belfroid et al. 1995)

depuration $t_{1/2} = 134$ d for high-dose treatment, $t_{1/2} = 153$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.168 2,3’,4,4’,5’,6-Hexachlorobiphenyl (PCB-168)

Chemical Name: 2,3’,4,4’,5’,6-hexachlorobiphenyl
Synonym: PCB-168, 2,3’,4,4’,5’,6-hexachloro-1,1’-biphenyl
CAS Registry No: 59291-65-5
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878

Melting Point (°C):
- 110–111 (Erickson 1986)
- 133 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
- 310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_fus (kJ/mol):

Entropy of Fusion, ΔS_fus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0134 (Sₐ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 5.72 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
- 9.76 × 10⁻⁴ (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 4.87 × 10⁻⁴ (Pₛ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 5.40 × 10⁻¹ (GC-RI correlation, Burkhard et al. 1985b)
- 6.88 × 10⁻⁴, 6.24 × 10⁻⁴ (supercooled liquid Pₛ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- log (Pₛ/P_a) = –4816/(T/K) + 12.99 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 13.07 (calculated-P/C, Burkhard 1984)
- 46.91 (calculated-QSAR-MCI X, Sabljc & Güsten 1989)
- 27.97 (calculated-QSAR, Dunnivant et al. 1992)
- 49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln Kₖₐₜ = –ΔH/RT + ΔS/R; R is the ideal gas constant, ΔH = 79 ± 18 kJ/mol, ΔS = 0.23 ± 0.06 kJ/mol-K

Octanol/Water Partition Coefficient, log Kₙₐₜ:
- 6.76 (calculated-TSA, Burkhard 1984)
- 7.11 (calculated-TSA, Hawker & Connell 1988a)
- 7.23, 7.13; 6.76, 6.71 (multi-column HPLC-k’ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 7.18, 6.74 (quoted average values from Risby et al. 1990, Sangster 1993)
- 7.17 (recommended, Hansch et al. 1995)
- 6.8539 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:
10.39 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

6.56 (suspended particulate matter, Burkhard 1984)
5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calc-molecular connectivity indices, Sabljie et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\text{1/2}$:
Volatile:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29–60$ d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:
7.1.1.169 3,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-169)

Common Name: 3,3′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-169, 3,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 32774-16-6
Molecular Formula: C₁₂H₄Cl₆
Molecular Weight: 360.878
Melting Point (°C):
201–202.0 (Hutzinger et al. 1974)
201 (Brodsky & Ballschmiter 1988)
Boiling Point (°C): 
Density (g/cm³):
Molar Volume (cm³/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔHₜₘ (kJ/mol):
Entropy of Fusion, ΔSₜₘ (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSₜₘ = 56 J/mol K), F:
0.0178 (calculated, Mackay et al. 1992; Passivirta et al. 1999)
0.0177 (Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
4.54 × 10⁻⁴, 3.0 × 10⁻⁴, 5.22 × 10⁻⁴, 9.07 × 10⁻⁴ (RP-HPLC-k correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0000219; 0.000116 (generator column-GC, ECD; estimated, Hong & Qiao 1995)
log (Sk/(mol/L)) = – 1.12 + 1403/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.000130 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000053, 0.000083, 0.000130, 0.000215 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.08 × 10⁻⁶ (GC-RI correlation, Burkhard et al. 1985a)
5.36 × 10⁻³ (supercooled liquid Pₜ, GC-RI correlation, Burkhard et al. 1985b)
6.76 × 10⁻³ (supercooled liquid Pₜ, GC-RI correlation, Fischer et al. 1992)
log (Pₜ/Pa) = – 5313/(T/K) + 13.64 (supercooled liquid Pₜ, GC-RT correlation, Falconer & Bidleman 1994)
1.03 × 10⁻⁴, 1.82 × 10⁻⁶ (supercooled liquid Pₜ, solid Pₛ, Passivirta et al. 1999)
log (Pₛ/Pₜ) = 16.59 – 6715/(T/K) (solid, Passivirta et al. 1999)
log (Pₛ/Pₜ) = 13.64 – 5313/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
1.57 (calculated-P/C, Burkhard et al. 1985b)
5.98 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
6.60 (calculated-QSPR, Dunnivant et al. 1992)
0.85 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
23.4 (from 11°C expstl. data and compensation point, Bamford et al. 2002)
ln Kₜₘ = ΔHₛ/RT + ΔSₛ/R; R is the ideal gas constant, ΔHₛ = 162 ± 20 kJ/mol, ΔSₛ = 0.51 ± 0.07 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:

7.42, 7.54, 7.62, 7.61 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.408 ± 0.005 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.39, 7.55; 7.46, 7.42 (multi-column HPLC-k’ correlation; capillary GC-RT correlation, different stationary phases, Risby et al. 1990)
7.55 (recommended, Sangster 1993)
7.41 (recommended, Hansch et al. 1995)
7.01 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or indicated:

12.51, 11.32; 11.19 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
11.27 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.97; 7.50 (22°C, zebrafish: log BCF$_w$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)
5.97, 7.51 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:

6.60 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}$(calc) = (0.16 – 0.5) × 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau$(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 7200$ d$^{-1}$; $k_2 = 0.00766$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_1 = 2$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03$ d$^{-1}$ (earthworm, Wågman et al. 2001)
$k_1 = 0.0065$ d$^{-1}$ with $t_\frac{1}{2} = 107$ d (newly contaminated oysters, Gardinali et al. 2004)
$k_2 = 0.0082$ d$^{-1}$ with $t_\frac{1}{2} = 85$ d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);
$t_{\frac{1}{2}} = 6000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation $t_{\frac{1}{2}} = 548$ min when irradiated in a TiO$_2$ semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
$t_{\frac{1}{2}} = 120000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Groundwater:

Sediment: $t_{\frac{1}{2}} = 165000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{\frac{1}{2}} = 165000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{\frac{1}{2}} = 24$ d in earthworm given contaminated food (Wågman et al. 2001)
Depuration $t_{\frac{1}{2}} = 107$ d for newly contaminated oysters, and $t_{\frac{1}{2}} = 85$ d for chronically contaminated oysters (Gardinial et al. 2004)
7.1.1.170 2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB-170)

Common Name: 2,2',3,3',4,4',5-Heptachlorobiphenyl
Synonym: PCB-170, 2,2',3,3',4,4',5-heptachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',4,4',5-heptachlorobiphenyl
CAS Registry No: 35065-30-6
Molecular Formula: C$_{12}$H$_{3}$Cl$_{7}$
Molecular Weight: 395.323
Melting Point (°C): 135 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$: 0.0833 (mp at 135°C)
Water Solubility (g/m$^3$ or mg/L at 25°C):
0.00767 (supercooled liquid $S_L$, Burkhard et al. 1985b)
0.00347 (20°C, supercooled liquid $S_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.000504 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.000395 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00052 (calculated-MCI $\chi$, Patil 1991)
0.000130 (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.37 × 10$^{-5}$ (supercooled liquid $P_L$, GC-RT correlation, Bidleman 1984)
3.37 × 10$^{-5}$ (GC-RI correlation, Burkhard et al. 1985a)
3.72 × 10$^{-4}$ (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
8.37 × 10$^{-5}$, 8.11 × 10$^{-5}$ (supercooled liquid $P_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.32 × 10$^{-3}$ (20°C, supercooled liquid $P_L$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.13 × 10$^{-3}$, 7.76 × 10$^{-3}$ (supercooled liquid $P_L$, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log ($P_L$/Pa) = – 5139/(T/K) + 13.07 (supercooled liquid, GC-RT correlation, Falconnor & Bidleman 1994)
Henry’s Law Constant (Pa m$^3$/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
19.25 (calculated-P/C, Burkhard 1985b)
1.52 (20°C, calculated-P/C, Murphy et al. 1987)
0.912 (wetted-wall column-GC, Brunner et al. 1990)
8.85 (calculated-QSPR, Dunnivant et al. 1992)
0.128, 0.760, 4.139, 20.84* ± 0.80, 78.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln $K_{AW} = 61.342 – 19725.76/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(164.0/\text{kJ/mol}^{-1}/RT) + (0.510/\text{kJ/mol}^{-1} \cdot \text{K}^{-1})/R]$; where $R = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
19.4 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R$; $R$ is the ideal gas constant, $\Delta H_{\text{f}} = 164 \pm 9 \text{ kJ/mol}$, $\Delta S_{\text{f}} = 0.51 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 7.05 (calculated-TSA, Burkhard 1984)
- 7.08 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
- 7.27 (calculated-TSA, Hawker & Connell 1988a)
- 7.03 (calculated-MCI $\chi$, Patil 1991)
- 7.30 (calculated-TSA, Murray & Andren 1992)
- 6.83 (generator column-GC, Larsen et al. 1992)
- 6.96 (recommended, Sangster 1993)
- 7.10 (estimated, Girvin & Scott 1997)
- 7.0639 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{OA}$ at $25^\circ$C or as indicated:
- 11.42 (10°C, estimated, Thomas et al. 1998)
- 12.34, 11.07; 11.02 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.69 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- 2.43–4.76 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 3.75–4.61 (Various marine species, mean lipid-normalized BCF, Hope et al. 1999)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.85 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.63, 5.48, 5.42, 4.99 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_{so}$, Lara & Ernst 1989)
- 5.632, 5.675 (marine humic substances of 5 mg/L DOC, quoted; calculated-MCI $\chi$, reported as association coefficient log $K_{so}$, Sabljic et al. 1989)
- 6.10 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 6.60 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 0.004$ d$^{-1}$ with $t_{1/2} = 164$ d ($8^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 180$ d ($8^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 164$ d for high-dose treatment, $t_{1/2} = 180$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment ($8^\circ$C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.171 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl (PCB-171)

Common Name: 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl
Synonym: PCB-171, 2,2′,3,3′,4,4′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6-heptachlorobiphenyl
CAS Registry No: 52663-71-5
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323

Melting Point (°C):
117.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.29 (Miller et al. 1984; Ruelle et al. 1993)
22.80 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):
51.04 (Miller et al. 1984; Shiu & Mackay 1986)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.124 (mp at 117.5°C)
0.109 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00624 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00217 (generator column-GC/ECD, Miller et al. 1984,1985)
0.00412 (20°C, supercooled liquid S, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
9.81 × 10⁻⁶ (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
0.00102, 0.000687, 0.000521 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87 × 10⁻⁴, 2.98 × 10⁻⁴ (supercooled liquid P, GC-RT correlation, different stationary phases, Bidleman 1984)
5.71 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985a)
4.69 × 10⁻⁴ (supercooled liquid P, GC-RI correlation, Burkhard et al. 1985b)
2.57 × 10⁻⁴, 3.17 × 10⁻⁴ (supercooled liquid P, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.73 × 10⁻⁴, 2.50 × 10⁻⁴ (selected, solid P; supercooled liquid P, Shiu & Mackay 1986)
1.26 × 10⁻⁴, 2.09 × 10⁻⁴ (supercooled liquid P, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{0}/Pa) = − 5008/(T/K) + 13.07 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
29.79 (calculated-P/C, Burkhard et al. 1985b)
5.40 (calculated-P/C, Shiu & Mackay 1986)
17.49 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln \( K_{AW} = -\Delta H_f/RT + \Delta S_f/R; R \) is the ideal gas constant, \( \Delta H_f = 101 \pm 9 \text{ kJ/mol, } \Delta S_f = 0.31 \pm 0.03 \text{ kJ/mol-K} \)
(Bamford et al. 2002)—see Comment by Goss et al. 2004


Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C or as indicated and reported temperature dependence equations: 9.50 (calculated- \( K_{ow}/K_{aw} \), Wania & Mackay 1996) 10.51 (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996) 12.31, 11.78, 11.14, 10.51, 9.96 (-10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995) \log K_{oa} = -5.71 + 4757/(T/K); (temp range -10 to 30°C, Harner & Bidleman 1996) 11.76, 10.51; 10.50 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999) 10.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \): 6.94 (suspended particulate matter, calculated- \( K_{ow} \), Burkhard 1984) 5.516 (marine humic substances of 5 mg/L DOC, reported as association coefficient log \( K_a \), calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\text{1/2} \): Volatilization: Photolysis: Hydrolysis: Oxidation: Biodegradation: Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
\( k_1 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 156 \text{ d} (8°C, \text{ juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004}) \)
\( k_1 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 182 \text{ d} (8°C, \text{ juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004}) \)

Half-Lives in the Environment:
Air: Surface water: Groundwater: Sediment: Soil: Biota: \( t_{1/2} = 260 \text{ d in worms at 8°C (Oliver 1987c).} \)
depuration \( t_{1/2} = 156 \text{ d for high-dose treatment, } t_{1/2} = 182 \text{ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004}) \)
**Polychlorinated Biphenyls (PCBs)**

### 7.1.1.172 2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB-172)

![Structure of 2,2',3,3',4,5,5'-Heptachlorobiphenyl](image)

**Common Name:** 2,2',3,3',4,5,5'-Heptachlorobiphenyl  
**Synonym:** PCB-172, 2,2',3,3',4,5,5'-heptachloro-1,1'-biphenyl  
**Chemical Name:** 2,2',3,3',4,5,5'-heptachlorobiphenyl  
**CAS Registry No:** 52663-74-8  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{3}Cl\textsubscript{7}  
**Molecular Weight:** 395.323  
**Melting Point (°C):** 113  
(estimated, Abramowitz & Yalkowsky 1990)  
**Boiling Point (°C):** (calculated-Le Bas method at normal boiling point)  
**Density (g/cm\textsuperscript{3}):** 330.9  
**Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):**  
**Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), F:**

**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):**  
- 0.00688 (\(S_L\), supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
- 0.00430 (20°C, supercooled liquid, Murphy et al. 1987)  
- 3.14 \times 10\textsuperscript{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)  
- 4.98 \times 10\textsuperscript{-4} (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
- 5.55 \times 10\textsuperscript{-4} (\(P_L\), supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
- 6.14 \times 10\textsuperscript{-4} (GC-RI correlation, Burkhard et al. 1985b)  
- 1.41 \times 10\textsuperscript{-4} (supercooled liquid \(P_L\), GC-RI correlation, Fischer et al. 1992)  
\[\log (P_L/Pa) = -5109/(T/K) + 12.28\] (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):  
- 31.82 (calculated-P/C, Burkhard 1984)  
- 1.317 (wetted wall column-GC/ECD, Brunner et al. 1990)  
- 12.07 (calculated-QSPR, Dunnivant et al. 1992)  
- 28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\[\ln K_{AW} = -\Delta H_{H}/RT + \Delta S_{H}/R; \ R \text{ is the ideal gas constant, } \Delta H_{H} = 149 \pm 13 \text{ kJ/mol, } \Delta S_{H} = 0.46 \pm 0.04 \text{ kJ/mol·K}\] (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):  
- 7.10 (calculated-TSA, Burkhard 1984)  
- 7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)  
- 6.85 (generator column-GC, Larsen et al. 1992)  
- 7.03 (recommended, Sangster 1993)  
- 7.2349 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\) at 25°C or as indicated:  
- 11.84, 10.67 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)  
- 10.50 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.89 (suspended particulate matter, Burkhard 1984)
- 5.71, 5.44, 5.38, 4.97 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_h$, Lara & Ernst 1989)
- 5.711; 5.66 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_h$, observed; calculated-MCI $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 165 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 179 \text{ d}$ ($8^\circ\text{C}$, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 165 \text{ d}$ for high-dose treatment, $t_{1/2} = 179 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment ($8^\circ\text{C}$, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.173 2,2′,3,3′,4,5,6-Heptachlorobiphenyl (PCB-173)

Common Name: 2,2′,3,3′,4,5,6-Heptachlorobiphenyl
Synonym: PCB-173, 2,2′,3,3′,4,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6-heptachlorobiphenyl
CAS Registry No: 68194-16-1
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C):
145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00731 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00416 (20°C, supercooled liquid, Murphy et al. 1987)
6.265 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
5.55 × 10⁻⁵ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.14 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m³/mol at 25°C):
29.89 (calculated-P/C, Burkhard 1984)
1.42 (wetted wall column-GC/ECD, Brunner et al. 1990)
18.48 (calculated-QSPR, Dunnivant et al. 1992)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 101 ± 9 kJ/mol, ΔS_{fus} = 0.31 ± 0.03 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
7.07 (calculated-TSA, Burkhard 1984)
7.02 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.30 (calculated-TSA, Murray & Andren 1992)
6.9556 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.79, 10.60 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
10.48 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.87 (suspended particulate matter, Burkhard 1984)
- 5.532 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 2$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 20 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)
- depuration $t_{1/2} = 162 \text{ d}$ for high-dose treatment, $t_{1/2} = 186 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.174 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl (PCB-174)

Common Name: 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl
Synonym: PCB-174, 2,2′,3,3′,4,5,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6′-heptachlorobiphenyl
CAS Registry No: 38411-25-5
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C):
130.6 (Burkhard 1985b)
Boiling Point (°C): 130.6 (Burkhard 1985b)
Density (g/cm³):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (KJ/mol):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), F: 0.092 (mp at 130.6°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00625 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00525 (20°C, supercooled liquid, Murphy et al. 1987)
0.001016 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.687 × 10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
3.191 × 10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.206 × 10^{-4} (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.19 × 10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.80 × 10^{-4}, 2.43 × 10^{-4} (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.69 × 10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
2.75 × 10^{-4} (supercooled liquid P_{L}, GC-RI correlation, Fischer et al. 1992)
log (P_{L}/Pa) = -4962/(T/K) + 12.90 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
93.53 (calculated-P/C, Burkhard 1984)
4.96 (20°C, calculated-P/C, Murphy et al. 1987)
1.419 (wetted wall column-GC/ECD, Brunner et al. 1990;)
17.13 (calculated-QSPR, Dunnivant et al. 1992)
4.91 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = -\Delta H_{\text{ fus}}/RT + \Delta S_{\text{ fus}}/R; R is the ideal gas constant, $\Delta H_{\text{ fus}} = 113 \pm 11$ kJ/mol, $\Delta S_{\text{ fus}} = 0.35 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{ow}$:
7.14 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:
- 11.67, 10.51; 10.64 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.38 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_{B}$:

Biota Sediment Accumulation Factor, BSAF:
- 89 (trout in Lake Ontario, Niimi 1996)
- 0.29, 2.8, 1.4 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, $\log K_{OC}$:
- 6.94 (suspended particulate matter, Burkhard 1984)
- 5.52 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_{a}$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 5.82 (Ispra soil, shake flask-GC, Pava-Perez et al. 1991)
- 6.60 (soil-organic carbon, calculated-$K_{OW}$, Girvin & Scott 1979)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration experiment - high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 194$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration experiment - high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
  - Biota: depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 194$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.175 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl (PCB-175)

![Chemical Structure](image)

**Common Name:** 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl  
**Synonym:** PCB-175, 2,2′,3,3′,4,5′,6-heptachloro-1,1′-biphenyl  
**Chemical Name:** 2,2′,3,3′,4,5′,6-heptachlorobiphenyl  
**CAS Registry No:** 40186-70-7  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{3}Cl\textsubscript{7}  
**Molecular Weight:** 395.323  
**Melting Point (°C):**  
133° (estimated, Abramowitz & Yalkowsky 1990)  
**Boiling Point (°C):**  
**Density (g/cm\textsuperscript{3}):**  
330.9 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):**  
**Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K):**  
Fugacity Ratio at 25°C (assuming ΔS\textsubscript{fus} = 56 J/mol K), F:  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):**  
0.00557 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)  
0.00894 (20°C, supercooled liquid, Murphy et al. 1987)  
0.00104 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)  
4.98 × 10\textsuperscript{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
7.00 × 10\textsuperscript{-4} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)  
7.72 × 10\textsuperscript{-4} (GC-RI correlation, Burkhard et al. 1985b)  
3.98 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}, GC-RI correlation, Fischer et al. 1992)  
\log (P\textsubscript{L}/P\textsubscript{a}) = –4962/(T/K) + 12.22 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)  
**Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):**  
49.55 (calculated-P/C, Burkhard 1984)  
22.63 (calculated-QSPR, Dunnivant et al. 1992)  
2.069 (calculated-QSPR, Achman et al. 1993)  
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)  
\ln K\textsubscript{AW} = –\Delta H\textsubscript{fus}/RT + \Delta S\textsubscript{fus}/R; R is the ideal gas constant, \Delta H\textsubscript{fus} = 101 ± 9 kJ/mol, \Delta S\textsubscript{fus} = 0.31 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004  
**Octanol/Water Partition Coefficient, log K\textsubscript{ow}:**  
7.19 (calculated-TSA, Burkhard 1984)  
6.92 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988a)  
6.92 (recommended, Sangster 1993)  
7.10 (estimated, Girvin & Scott 1997)  
7.0957 (calculated-molecular properties MNDO-AM1 method, Makino 1998)  
**Octanol/Air Partition Coefficient, log K\textsubscript{oa} at 25°C or as indicated:**  
11.35, 10.17 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)  
10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Biota Sediment Accumulation Factor, BSAF:
- 144 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.99 (suspended particulate matter, Burkhard 1984)
- 5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.60 (soil-organic carbon, calculated-$K_{OW}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Biocaccumulation and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_2 = 0.005 \text{ d}^{-1}$ with $t_\frac{1}{2} = 154 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_\frac{1}{2} = 169 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:

Biota: depuration $t_\frac{1}{2} = 154 \text{ d}$ for high-dose treatment, $t_\frac{1}{2} = 169 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.176 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl (PCB-176)

Cl Cl Cl Cl Cl
\[
\text{Cl} \quad \text{Cl} \quad \text{Cl} \\
\text{Cl} \quad \text{Cl} \quad \text{Cl}
\]

Common Name: 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl
Synonym: PCB-176, 2,2′,3,3′,4,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-65-7
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.00601 (Sℓ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 0.00585 (20°C, supercooled liquid, Murphy et al. 1987)
- 0.00280 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
- 0.00314 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 1.52 × 10⁻³ (Pℓ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 1.66 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985b)
- 5.31 × 10⁻⁴, 8.83 × 10⁻⁴ (supercooled liquid Pℓ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 1.35 × 10⁻⁵ (20°C, supercooled liquid, Murphy et al. 1987)
- \( \log (P/\text{mmHg}) = 11.50 – 5080/(T/K) \) (GC-RT correlation, Tateya et al. 1988)
- 4.17 × 10⁻⁴, 7.24 × 10⁻⁴ (supercooled liquid Pℓ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
- \( \log (P_{\text{f}}/\text{Pa}) = -4579/(T/K) + 12.07 \) (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 100 (calculated-P/C, Burkhard 1984)
- 9.12 (20°C, calculated-P/C, Murphy et al. 1987)
- 30.11 (calculated-QSPR, Dunnivant et al. 1992)
- 3.13 (calculated-QSPR, Achman et al. 1993)
- 107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\( \ln K_{\text{AW}} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R; \) R is the ideal gas constant, \( \Delta H_{\text{f}} = 62 ± 5 \text{ kJ/mol, } \Delta S_{\text{f}} = 0.18 ± 0.02 \text{ kJ/mol-K} \) (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
- 7.16 (calculated-TSA, Burkhard 1984)
- 6.55 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
- 6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.76 (generator column-GC, Larsen et al. 1992)
- 6.65 (recommended, Sangster 1993)
- 6.6653 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

- 11.22, 10.06; 10.13 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.96 (suspended particulate matter, Burkhard 1984)
- 5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-
molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 184 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration
  expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration
  expt.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 184 \text{ d}$ for high-dose treatment, $t_{1/2} = 153 \text{ d}$ for high-dose + enzyme CYP1A-inducing
  compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.177 2,2’,3,3’,4,5’,6’-Heptachlorobiphenyl (PCB-177)

```
Cl     Cl     Cl     Cl     Cl
|     |     |     |     |     |
|     |     |     |     |     |
|     |     |     |     |     |
Cl     Cl
```

Common Name: 2,2’,3,3’,4,5’,6’-Heptachlorobiphenyl
Synonym: PCB-177, 2,2’,3,3’,4,5’,6’-heptachloro-1,1′-biphenyl
Chemical Name: 2,2’,3,3’,4,5’,6’-heptachlorobiphenyl
CAS Registry No: 52663-70-4
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00656 (S_l supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00482 (20°C, supercooled liquid, Murphy et al. 1987)
0.00150 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
4.98 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.40 × 10⁻⁴ (P_l supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.88 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
2.50 × 10⁻⁴, 3.38 × 10⁻⁴ (supercooled liquid P_l, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.15 × 10⁻⁵ (20°C, supercooled liquid, Murphy et al. 1987)
1.38 × 10⁻⁴, 2.51 × 10⁻⁴ (supercooled liquid P_l; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_l/Pa) = –4962/(T/K) + 13.04 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa-m³/mol at 25°C or as indicated):
26.45 (calculated-P/C, Burkhard 1984)
3.34 (20°C, calculated-P/C, Murphy et al. 1987)
15.55 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
5.12 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
50.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{l}/RT + ΔS_{l}/R; R is the ideal gas constant, ΔH_{l} = 112 ± 11 kJ/mol, ΔS_{l} = 0.34 ± 0.04 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
7.12 (calculated-TSA, Burkhard 1984)
6.73 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.73 (recommended, Sangster 1993)
October/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:
- 11.74, 10.58 (0, 20°C, multi-column GC-k correlation, Zhang et al. 1999)
- 10.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:
- 6.92 (suspended particulate matter, Burkhard 1984)
- 5.54, 5.39, 5.35, 4.90 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 5.359; 5.52 (marine humic substances with 5 mg/L of DOC, reported as association coefficient $\log K_h$, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
- 5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 6.60 (soil-organic carbon, calculated-$K_{OW}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.005 \, d^{-1}$ with $t_{1/2} = 147 \, d$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
  - $k_2 = 0.004 \, d^{-1}$ with $t_{1/2} = 186 \, d$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 147 \, d$ for high-dose treatment, $t_{1/2} = 186 \, d$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.178 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl (PCB-178)

Common Name: 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-178, 2,2′,3,3′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-67-9
Molecular Formula: C₁₂H₃Cl₇
Molecular Weight: 395.323
Melting Point (°C):
125 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00588 (S₁, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00884 (20°C, supercooled liquid, Murphy et al. 1987)
0.001016 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.000627 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.57 × 10⁻⁴ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.24 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
1.47 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.70 – 5220/(T/K) (GC-RT correlation, Tateya et al. 1988)
4.57 × 10⁻⁴ (supercooled liquid P₁, GC-RI correlation, Fischer et al. 1992)
log (P₁/Pa) = –4962/(T/K) + 13.28 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
44.08 (calculated-P/C, Burkhard 1984)
6.586 (20°C, calculated-P/C, Murphy et al. 1987)
2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)
21.61 (calculated-QSPR, Dunnivant et al. 1992)
11.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
71.4 (from 11°C expit. data and compensation point, Bamford et al. 2002)
$\ln K_{\text{AW}} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R$; R is the ideal gas constant, $\Delta H_{\text{f}} = 90 ± 10$ kJ/mol, $\Delta S_{\text{f}} = 0.27 ± 0.03$ kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
7.17 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.85 (recommended, Sangster 1993)
7.0564 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated:
- 11.28, 10.12 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log \( BCF \) or log \( K_b \):

Sorption Partition Coefficient, log \( K_{OC} \):
- 6.97 (suspended particulate matter, Burkhard 1984)
- 5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log \( K_a \), calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
  - \( k_2 = 0.004 \text{ d}^{-1} \) with \( t_{\frac{1}{2}} = 156 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - \( k_2 = 0.004 \text{ d}^{-1} \) with \( t_{\frac{1}{2}} = 166 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration \( t_{\frac{1}{2}} = 156 \text{ d} \) for high-dose treatment, \( t_{\frac{1}{2}} = 166 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.179 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl (PCB-179)

Common Name: 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-179, 2,2′,3,3′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-64-6
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³): 330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00632 (S_ł, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00454 (RP-HPLC-k′ correlation, Brodsky & Ballischmiter 1988)
0.0039 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.42 × 10⁻³ (P_L, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.55 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985b)
5.15 × 10⁻⁴, 1.004 × 10⁻³ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.01 × 10⁻⁴, 8.71 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P/P_a) = −4579/(T/K) + 12.07 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
88.96 (calculated-P/C, Burkhard 1984)
2.432 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.91 (calculated-QSPR, Dunnivant et al. 1992)
37.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 144 ± 7 kJ/mol, ΔS_{f} = 0.45 ± 0.03 kJ/mol-K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
6.77, 8.13 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
7.14 (calculated-TSA, Burkhard 1984)
6.41 (RP-HPLC-k′ correlation, Brodsky & Ballischmiter 1988)
6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.41 (recommended, Sangster 1993)
6.6366 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
  11.26, 10.10 (0, 20°C, multi-column $k'$ correlation, Zhang et al. 1999)
  10.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
  6.94 (suspended particulate matter, Burkhard 1984)
  5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calculated-
molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration
  expt.- high-dose treatment, Buckman et al. 2004)
  $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 198 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration
  expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
  Air:
  Surface water:
  Ground water:
  Sediment:
  Soil:
  Biota: depuration $t_{1/2} = 171 \text{ d}$ for high-dose treatment, $t_{1/2} = 198 \text{ d}$ for high-dose + enzyme CYPIA-inducing
  compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.180 2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180)

Common Name: 2,2',3,4,4',5,5'-Heptachlorobiphenyl
Synonym: PCB-180, 2,2',3,4,4',5,5'-heptachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,4',5,5'-heptachlorobiphenyl
CAS Registry No: 35065-29-3
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 109–110 (Hutzinger et al. 1974)
Boiling Point (°C): 240–280 (20mm Hg)
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.144 (calculated-Mackay et al. 1992; Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
0.00656 (supercooled liquid S_{L}, calculated-TSA, Burkhard et al. 1985b)
0.00385 (20°C, supercooled liquid S_{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00031 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
0.00063 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00053 (calculated-MCI χ_{P}, Patil 1991)
2.45 × 10⁻⁴ (calculated-QSPR, Dunnivant et al. 1992)
log S_{L} (mol/L) = −1.676 + 1132/(T/K) (supercooled liquid, Passivirta et al. 1999)
3.17 × 10⁻³; 5.22 × 10⁻³ (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
log S_{L}/(mol m⁻³) = −1356/(T/K) – 0.33 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.10 × 10⁻³ (Verlag Chemie 1983)
1.30 × 10⁻⁴, 1.29 × 10⁻⁴ (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Bidleman 1984)
8.07 × 10⁻⁵ (GC-R1 correlation, Burkhard et al. 1985a)
5.06 × 10⁻⁴ (supercooled liquid P_{L}, calculated-GC-R1 correlation, Burkhard 1985b)
1.21 × 10⁻⁴, 1.43 × 10⁻⁴ (supercooled liquid. P_{L}, GC-RT correlation, different stationary phases Foreman & Bidleman 1985)
3.14 × 10⁻⁵ (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
8.13 × 10⁻⁵, 1.20 × 10⁻⁴ (supercooled liquid P_{L}, GC-R1 correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = −5042/(T/K) + 13.03 (GC-RT correlation, Falconer & Bidleman 1994)
1.45 × 10⁻⁴, 2.09 × 10⁻⁴ (supercooled liquid P_{L}, solid P_{S}, Passivirta et al. 1999)
log (P_{L}/Pa) = 15.98 – 6173/(T/K) (solid, Passivirta et al. 1999)
log (P_{L}/Pa) = 13.03 – 5042/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.32 × 10⁻⁴; 1.072 × 10⁻⁴ (supercooled P_{L}; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_{L}/Pa = −4809/(T/K) + 12.16 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)
Henry’s Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- log H/(Pa m³/mol) = 14.71 – 3910/(T/K) (Passivirta et al. 1999)
- log H/(Pa m³/mol) = –3453/(T/K) + 12.49 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

- 7.12 (calculated-TSA, Burkhard 1984)
- 6.70 (calculated-chlorine substituents, Oliver 1987a)
- 7.21 (RP-HPLC-k′ correlation, Brodsky & Ballischmiter 1988)
- 7.02 (calculated-MCI χ, Patil 1991)
- 7.40 (calculated-TSA, Murray & Andren 1992)
- 6.56 (average, generator column-GC, Larsen et al. 1992)
- 6.89 (recommended, Sangster 1993)
- 7.2506 (calculated-molecular properties MNDO-AM1, Makino 1998)
- 7.20 (calculated, Passivirta et al. 1999)
- 7.29, 7.16 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K<sub>OA</sub> at 25°C or as indicated and reported temperature dependence equations:

- log K<sub>OA</sub> = –4.70 + 4535/(T/K); (temp range –10 to 30°C, Harner & Bidleman 1996)
- log K<sub>OA</sub> = –3.31 + 3930/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 11.22 (10°C, estimated, Thomas et al. 1998)
- 11.94, 10.72; 10.86 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
- 10.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 10.12, 10.16 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- log K<sub>OA</sub> = 4975/(T/K) – 6.55 (LDV linear regression of literature data, Li et al. 2003)
- log K<sub>OA</sub> = 4845/(T/K) – 6.09 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

- 2.99–5.68 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.22–6.41 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 4.45, 6.45 (Daphnia magna, 21-d exposure: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 6.06, 7.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K<sub>OC</sub> at 25°C or as indicated:

- 6.92 (suspended particulate matter, calculated-K<sub>OA</sub>, Burkhard 1984)
- 6.2–7.4, 6.9; 7.30 (suspended sediments, range; average, algae > 50 μm, Oliver 1987a)
- 6.51 (Lake Michigan water column, Swackhamer & Armstrong 1987)
5.73, 5.54, 5.50, 5.09 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_h$, Lara & Ernst 1989)

5.73; 5.66 (marine humic substances at 5 mg/L DOC, quoted; calculated-MCI $\chi$, reported as log $K_h$, Sabljic et al. 1989)

6.36, 6.23, 6.10 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

5.78 (Ispra soil, shake flask-GC/ECD, Paya-Perez et al. 1991)

6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

6.60 (soil, calculated-$K_{ow}$, Girvin & Scott 1997)

6.53–7.76; 5.80–7.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

5.42; 6.56, 7.42, 6.83 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

6.31–6.98 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Biocorcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 0.049 \text{ h}^{-1}$; $k_1 = 0.008 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)

$k_2 = 0.0246 \text{ d}^{-1}$ with an elimination $t_{1/2} = 282 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_2 = 0.00348 \text{ h}^{-1}$; $k_2 = 0.111 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1(\text{calc}) = 2 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2(\text{calc}) = 0.03 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

$k_2 = 0.021 \text{ d}^{-1}$ with $t_{1/2} = 33.0 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: $t_{1/2} = 12000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 240000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent, $t_{1/2} = 25 \text{ yr}$ (Geyer et al. 2000)

$S = 330000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 333000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} = 28.3 \text{ d}$ from earthworm (Belfroid et al. 1995);

elimination $t_{1/2} = 22 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration $t_{1/2} = 162 \text{ d}$ for high-dose treatment, $t_{1/2} = 186 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

depuration $t_{1/2} = 33.0 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004)
TABLE 7.1.1.180.1
Reported Henry's law constants and octanol-air partition coefficients of 2,2',3,4,4',5,5'-heptachlorobiphenyl (PCB-180) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-GC/MS</td>
<td>4°C, 0.425</td>
</tr>
<tr>
<td>11</td>
<td>2.025</td>
</tr>
<tr>
<td>18</td>
<td>8.96</td>
</tr>
<tr>
<td>25</td>
<td>37.0</td>
</tr>
<tr>
<td>31</td>
<td>118.5</td>
</tr>
</tbody>
</table>

\[
\ln K_{AW} = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}
\]
A: 53.7647 
B: 17272 

\[
\Delta H_{OA}/(kJ \cdot mol^{-1}) = 86.83
\]

enthalpy, entropy change:
\[
\Delta H/(kJ \cdot mol^{-1}) = 143.6 \pm 7.4
\]
\[
\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 447 \pm 26
\]

FIGURE 7.1.1.180.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',3,4,4',5,5'-heptachlorobiphenyl (PCB-180).
7.1.1.181 2,2′,3,4,4′,5,6-Heptachlorobiphenyl (PCB-181)

Common Name: 2,2′,3,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-181, 2,2′,3,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 74472-47-2
Molecular Formula: C₁₂H₃Cl₇
Molecular Weight: 395.323
Melting Point (°C): 140 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₜₜ (kJ/mol):
Entropy of Fusion, ΔSₘₜₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₜₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00625 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.44 × 10⁻⁴, 5.21 × 10⁻⁴, 2.30 × 10⁻⁴, 4.54 × 10⁻⁴ (RP-HPLC-k’ correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
3.95 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.44 × 10⁻⁴ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.11 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
2.92 × 10⁻⁴, 4.206 × 10⁻⁴ (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54 × 10⁻⁴ (20°C, supercooled liquid, Murphy et al. 1987)
log (Pₗ/Pₐ) = –4962/(T/K) + 13.11 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
40.83 (calculated-P/C, Burkhard 1984)
23.31 (calculated-QSPR, Dunnivant et al. 1992)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₐₙₐ = –ΔHᵢ/RT + ΔSᵢ/R; R is the ideal gas constant, ΔHᵢ = 101 ± 9 kJ/mol, ΔSᵢ = 0.31 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₗₜₗ:\n7.14 (calculated-TSA, Burkhard 1984)
7.11, 7.12, 7.19, 7.11 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.13 (recommended, Sangster 1993)
7.0558 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log Kₗₜₐ:\n10.61 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log $K_B$ or log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.94 (suspended particulate matter, Burkhard 1984)
- 5.516 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:
7.1.1.182 2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-182)

Common Name: 2,2',3,4,4',5,6'-Heptachlorobiphenyl
Synonym: PCB-182, 2,2',3,4,4',5,6'-heptachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,4',5,6'-heptachlorobiphenyl
CAS Registry No: 60145-23-5
Molecular Formula: C$_{12}$H$_3$Cl$_7$
Molecular Weight: 395.323
Melting Point (°C):
152 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):

Density (g/cm$^3$):
330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH$_{fus}$ (kJ/mol):
Entropy of Fusion, ΔS$_{fus}$ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS$_{fus}$ = 56 J/mol K), F: 0.0567 (mp at 152°C)

Water Solubility (g/m$^3$ or mg/L at 25°C):
5.34 × 10$^{-3}$ (S$_L$ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
8.26 × 10$^{-4}$ (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
3.95 × 10$^{-4}$ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.36 × 10$^{-4}$ (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.31 × 10$^{-3}$ (P$_L$ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.43 × 10$^{-3}$ (GC-RI correlation, Burkhard et al. 1985b)
3.66 × 10$^{-4}$, 3.56 × 10$^{-4}$ (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.14 × 10$^{-4}$, 3.72 × 10$^{-4}$ (supercooled liquid P$_L$: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P$_L$/Pa) = –4962/(T/K) + 13.11 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
97.07 (calculated-P/C, Burkhard 1984)
26.04 (calculated-QSPR, Dunnivant et al. 1992)
2.07 (calculated-QSPR, Achman et al. 1993)
8.71 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
63.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

ln K$_{AW}$ = –ΔH$_{f}$/RT + ΔS$_{f}$/R; R is the ideal gas constant, ΔH$_{f}$ = 97 ± 10 kJ/mol, ΔS$_{f}$ = 0.30 ± 0.04 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K$_{OW}$:
7.22 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
7.0964 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$:
10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
7.02 (suspended particulate matter, Burkhard 1984)
5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calc-molecular connectivity indices, Sabljic et al. 1989)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_2 = 0.004 \text{d}^{-1}$ with $t_{1/2} = 159 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp. high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{d}^{-1}$ with $t_{1/2} = 182 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp. high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:

Biota: depuration $t_{1/2} = 159 \text{ d}$ for high-dose treatment, $t_{1/2} = 182 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.183 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl (PCB-183)

Common Name: 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-183, 2,2′,3,4,4′,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-69-1
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C):
152 (estimated, Abramowitz & Yalkowsky 1990)
83 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.270 (mp at 83°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00534 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00490 (20°C, supercooled liquid, Murphy et al. 1987)
3.14 × 10⁻⁴, 4.98 × 10⁻⁴, 6.27 × 10⁻⁴, 5.09 × 10⁻⁴ (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.14 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000641 (calculated-group contribution method, Kühne et al. 1995)
9.27 × 10⁻⁴, 2.49 × 10⁻³ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.77 × 10⁻³ (calculated-mp and K_{OW}, Ran et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.38 × 10⁻⁴ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.05 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
3.57 × 10⁻⁴, 5.09 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
8.61 × 10⁻⁵ (20°C, supercooled liquid, Murphy et al. 1987)
2.0 × 10⁻⁴, 3.24 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = –4962/(T/K) + 13.19 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
47.32 (calculated-P/C, Burkhard 1984)
6.89 (20°C, calculated-P/C, Murphy et al. 1987)
20.40 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
0.326, 0.954 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
61.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = –ΔH_{fus}/RT + ΔS_{fus}/R; R is the ideal gas constant, ΔH_{fus} = 100 ± 10 kJ/mol, ΔS_{fus} = 0.30 ± 0.04 kJ/mol K
(Bamford et al. 2002)—see Comment by Goss et al. 2004

© 2006 by Taylor & Francis Group, LLC
Octanol/Water Partition Coefficient, log $K_{OW}$:
7.22 (calculated-TSA, Burkhard 1984)
7.02, 7.13, 6.96, 7.07 (RP-HPLC-$k'$ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (generator column-GC, Larsen et al. 1992)
6.92 (recommended, Sangster 1993)
7.0868 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
8.27 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
10.80 (10°C, estimated, Thomas et al. 1998)
11.44, 10.26; 10.35 (0, 20°C, multi-column GC-$k'$ correlation; calculated at 20°C, Zhang et al. 1999)
10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
5.84, 7.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:
220 (trout in Lake Ontario, Niimi 1996)
0.52, 4.2, 0.84 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log $K_{OC}$:
7.02 (suspended particulate matter, Burkhard 1984)
5.53, 5.40, 5.35, 4.92 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_H$, Lara & Ernst 1989)
5.53; 5.50 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_H$, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
6.36, 6.25, 6.09 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
5.82 (Ispra soil, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

\[ k_2 = 0.004 \text{ d}^{-1} \text{ with } t_{1/2} = 165 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration experiment - high-dose treatment, Buckman et al. 2004)} \]

\[ k_2 = 0.003 \text{ d}^{-1} \text{ with } t_{1/2} = 206 \text{ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration experiment - high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)} \]

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{1/2} = 165$ d for high-dose treatment, $t_{1/2} = 206$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.184 2,2',3,4,4',6,6'-Heptachlorobiphenyl (PCB-184)

Common Name: 2,2',3,4,4',6,6'-Heptachlorobiphenyl
Synonym: PCB-184, 2,2',3,4,4',6,6'-heptachloro-1,1'-biphenyl
Chemical Name: 2,2',3,4,4',6,6'-heptachlorobiphenyl
CAS Registry No: 74472-48-3
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 108 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m^3 or mg/L at 25°C):
0.00514 (S_{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00198 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C):
1.65 × 10^{-3} (P_{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.80 × 10^{-3} (GC-RJ correlation, Burkhard et al. 1985b)
Henry’s Law Constant (Pa·m^3/mol at 25°C):
126.7 (calculated-P/C, Burkhard 1984)
46.42 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 62 ± 5 kJ/mol, ΔS_{f} = 0.18 ± 0.02 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
7.23 (calculated-TSA, Burkhard 1984)
6.76 (generator column-GC, Larsen et al. 1992)
6.65 (recommended, Sangster 1993)
6.8203 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa}:
10.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{wc}:
7.03 (suspended particulate matter, Burkhard 1984)
5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_{b}, calculated-molecular connectivity indices, Sabljic et al. 1989)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

\[ k_1 = 2 \text{ (food lipid mg)/(g worm lipid-d); \ } k_2 = 0.03 \text{ d}^{-1} \text{ (earthworm, Wågman et al. 2001)} \]

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:

Biota: elimination $t_{1/2} = 20$ d in earthworm given contaminated food (Wågman et al. 2001)
Polychlorinated Biphenyls (PCBs)

7.1.1.185 2,2′,3,4,5,5′,6-Heptachlorobiphenyl (PCB-185)

Common Name: 2,2′,3,4,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-185, 2,2,3,4,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52712-05-7
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 149 (Bruggeman et al. 1982; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.3702
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.0607 (mp at 149°C)
0.0595 (Mackay et al. 1980; Shiu & Mackay 1986)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.00047 (generator column-GC/ECD, Weil et al. 1974)
0.00546 (20°C, supercooled liquid S_{L}, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.71 × 10⁻⁴, 8.26 × 10⁻⁴, 6.27 × 10⁻⁴, 6.56 × 10⁻⁴ (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.75 × 10⁻³ (GC-RI correlation, Burkhard et al. 1985a)
7.28 × 10⁻¹ (supercooled liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)
3.21 × 10⁻¹, 4.78 × 10⁻¹ (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.70 × 10⁻¹, 2.95 × 10⁻¹ (supercooled liquid P_{L}; GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_{L}/Pa) = – 4962/(T/K) + 13.15 (supercooled liquid P_{L}, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
46.0 (calculated-P/C, Burkhard et al. 1985b)
1.62 (wetted-wall column-GC, Brunner et al. 1990)
21.71 (calculated-QSPR, Dunnivant et al. 1992)
2.67 (calculated-QSPR, Achman et al. 1993)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 101 ± 9 kJ/mol, ΔS_{f} = 0.31 ± 0.03 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{OW}:
7.93 (TLC-RT correlation, Bruggeman et al. 1982)
7.01, 6.98, 6.96, 7.00 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.99 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$:
- 10.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- 4.36 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
- 5.93; 7.46 (22°C, zebrafish: log BCF$_W$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)
- 5.93, 7.47 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
- 5.95 (Koch 1983)
- 6.94 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.52 (marine humic substances of 5 mg/L DOC, calculated-MCI $\chi$, reported as log $K_a$, Sabljic et al. 1989)
- 5.33 (calculated-$K_{OW}$, Bahnick & Doucette 1988)
- 6.43 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.28 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 6.29, 6.08, 6.13 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
- 5.80 (calculated-MCI, Park & Lee 1993)
- 6.50 (soil, calculated-$K_{OW}$, Girvin & Scott 1997)
- 6.40 (soil, calculated-universal solvation model; Winglet et al. 2000)

Sorption Partition Coefficient, log $K_{OM}$:
- 5.95, 5.31 (selected, calculated-molecular connectivity indices $\chi$, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
- Biodegradation:
- Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 5810$ d$^{-1}$; $k_2 = 0.00677$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 156$ d ($8^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 184$ d ($8^\circ$C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: $t_{1/2} = 48$ d in *Picea omorika* (Reischl et al. 1989 from Reischl 1988).
  depuration $t_{1/2} = 156$ d for high-dose treatment, $t_{1/2} = 184$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment ($8^\circ$C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.186 2,2′,3,4,5,6,6′-Heptachlorobiphenyl (PCB-186)

Common Name: 2,2′,3,4,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-186
Chemical Name: 2,2′,3,4,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74472-49-4
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C):
142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
330.9 (Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00672 (S sub L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00157 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.35 × 10⁻³ (P sub L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.47 × 10⁻³ (GC-R1 correlation, Burkhard et al. 1985b)
4.68 × 10⁻⁴, 7.55 × 10⁻⁴ (supercooled liquid P sub L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
\( \log (P_{L}/P_{a}) = -4579/(T/K) + 12.03 \) (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
79.13 (calculated-P/C, Burkhard 1984)
37.3 (calculated-QSPR, Dunnivant et al. 1992)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
\( \ln K_{AW} = -\Delta H_{f//RT} + \Delta S_{f//R} / R \); R is the ideal gas constant, \( \Delta H_{f//} = 62 \pm 5 \) kJ/mol, \( \Delta S_{f//} = 0.18 \pm 0.02 \) kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log \( K_{OW} \):
7.11 (calculated-TSA, Burkhard 1984)
6.69 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.7069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log \( K_{OA} \):
10.36 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log \( K_{B} \):
Sorption Partition Coefficient, log \( K_{OC} \):
6.91 (suspended particulate matter, Burkhard 1984)
5.383 (marine humic substances 5 mg/L of DOC, reported as association coefficient log \( K_{a} \), calculated-molecular connectivity indices, Sabljic et al. 1989)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
  - Volatilization:
  - Photolysis:
  - Photooxidation:
  - Hydrolysis:
  - Biodegradation:
  - Biotransformation:
  - Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
  - Air:
  - Surface water:
  - Ground water:
  - Sediment:
  - Soil:
  - Biota:
Polychlorinated Biphenyls (PCBs)

7.1.1.187 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl (PCB-187)

Common Name: 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-187, 2,2′,3,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-68-0
Molecular Formula: C\(_{12}\)H\(_3\)Cl\(_7\)
Molecular Weight: 395.323

Melting Point (°C):
- 149.0 (Mackay et al. 1980; Burkhard et al. 1985a)
- 147 (Ruelle & Kesselring 1997)

Boiling Point (°C):
- 417 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

Density (g/cm\(^3\)):
- 0.00451 (20°C, supercooled liquid S\(_L\), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 0.0826 (RP-HPLC-k′ correlation, Brodsky & Ballischminter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 3.05 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RT correlation, Bidleman 1984)
- 3.92 × 10\(^{-3}\) (GC-RI correlation, Burkhard et al. 1985a)
- 5.98 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RI correlation, Burkhard et al. 1985b)
- 3.47 × 10\(^{-4}\), 5.74 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 9.42 × 10\(^{-5}\) (20°C, supercooled liquid P\(_L\), calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- 2.14 × 10\(^{-4}\), 3.72 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RI correlation, different stationary phases, Fischer et al. 1992)
- log (P\(_L\)/Pa) = –4977/(T/K) + 12.96 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C or as indicated and reported temperature dependence equations):
- 42.15 (calculated-P/C, Burkhard et al. 1985b)
- 8.41 (20°C, calculated-P/C, Murphy et al. 1987)
- 20.55 (calculated-QSPR, Dunnivant et al. 1992)
- 2.07 (calculated-QSPR, Achman et al. 1993)
- 3.304, 8.72, 23.84, 82.20 ± 2.2, 136.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
- ln K\(_{AW}\) = 35.242 – 11582.87/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
- K\(_{AW}\) = \exp\{–(96.3/J·mol\(^{-1}\)·K\(^{-1}\))/RT\} + (0.293/J·mol\(^{-1}\)·K\(^{-1}\))/R\}; where R = 8.314 J·K\(^{-1}\)·mol\(^{-1}\) and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
- 65.9 (exptl. data, Bamford et al. 2002)
- ln K\(_{AW}\) = –\(\Delta H_i/RT + \Delta S_i/R\); R is the ideal gas constant, \(\Delta H_i = 96 ± 7\) kJ/mol, \(\Delta S_i = 0.29 ± 0.02\) kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, $\log K_{OW}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.19</td>
<td>calculated-TSA, Burkhard 1984</td>
</tr>
<tr>
<td>6.92</td>
<td>(RP-HPLC-RI correlation, Brodsky &amp; Ballschm 1988)</td>
</tr>
<tr>
<td>7.17</td>
<td>(calculated-TSA, Hawker &amp; Connell 1988a; quoted, Hansch et al. 1995)</td>
</tr>
<tr>
<td>7.40</td>
<td>(calculated-TSA, Murray &amp; Andren 1992)</td>
</tr>
<tr>
<td>6.76</td>
<td>(generator column-GC, Larsen et al. 1992)</td>
</tr>
<tr>
<td>6.84</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>7.10</td>
<td>(estimated, Girvin &amp; Scott 1997)</td>
</tr>
<tr>
<td>7.0464</td>
<td>(calculated-molar properties MNDO-AM1 method, Makino 1998)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.87; 9.25</td>
<td>(fugacity meter/generator column-GC; calculated, Kömp &amp; McLachlan 1997a)</td>
</tr>
<tr>
<td>$\log K_{OA} = -5.20 + 4490/(T/K)$</td>
<td>(fugacity meter, temp range 10–43°C, Kömp &amp; McLachlan 1997a)</td>
</tr>
<tr>
<td>10.85</td>
<td>(10°C, estimated, Thomas et al. 1998)</td>
</tr>
<tr>
<td>11.36, 10.22</td>
<td>(0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)</td>
</tr>
<tr>
<td>10.54</td>
<td>(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, $\log BCF$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method/Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.51–5.48</td>
<td>(various marine species, mean dry wt. BCF, Hope et al. 1998)</td>
</tr>
<tr>
<td>4.94–6.05</td>
<td>(various marine species, mean lipid-normalized BCF, Hope et al. 1998)</td>
</tr>
</tbody>
</table>

Biota Sediment Accumulation Factor, BSAF:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method/Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>244</td>
<td>(trout in Lake Ontario, Niimi 1996)</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, $\log K_{OC}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Method/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.99</td>
<td>(suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)</td>
</tr>
<tr>
<td>5.51, 5.40, 5.33, 4.90</td>
<td>(marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_{h}$, Lara &amp; Ernst 1989)</td>
</tr>
<tr>
<td>5.51; 5.50</td>
<td>(marine humic substances of 5 mg/L DOC, quoted; calculated-MCI $\chi$, reported as log $K_{OC}$, Sabljic et al. 1989)</td>
</tr>
<tr>
<td>6.60</td>
<td>(colloids and micro-particulates in precipitation events, GC/ECD, Murray &amp; Andren 1992)</td>
</tr>
<tr>
<td>6.60</td>
<td>(soil, calculated-$K_{OW}$, Girvin &amp; Scott 1997)</td>
</tr>
<tr>
<td>6.40; 6.00</td>
<td>(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- **Volatilization:**
- **Photolysis:**
- **Hydrolysis:**
- **Oxidation:**
- **Biodegradation:**
- **Biotransformation:**

**Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**

- $k_1 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 131 \text{ d}$ and $k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 71 \text{ d}$ for food concn of 22 ng/g and 125 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- $k_1 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 159 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 190 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
Half-Lives in the Environment:
  Air:
  Surface water:
  Groundwater:
  Sediment:
  Soil:
  Biota: depuration $t_{1/2} = 71–131$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
  depuration $t_{1/2} = 159$ d for high-dose treatment, $t_{1/2} = 190$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.188 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl (PCB-188)

Common Name: 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-188, 2,2′,3,4′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74487-85-7
Molecular Formula: C\textsubscript{12}H\textsubscript{3}Cl\textsubscript{7}
Molecular Weight: 395.323
Melting Point (°C):
130 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):

Density (g/cm\textsuperscript{3}):

Molar Volume (cm\textsuperscript{3}/mol):
330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):

Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):

Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
0.00538 (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00451 (20°C, supercooled liquid, Murphy et al. 1987)
0.00128 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
0.00125 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.55 \times 10^{-3} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55 \times 10^{-4}, 1.69 \times 10^{-3}, 2.96 \times 10^{-4} (P\textsubscript{L} supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI \(\chi\), Burkhard et al. 1985b)
8.51 \times 10^{-4}, 1.50 \times 10^{-3} (supercooled liquid P\textsubscript{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.42 \times 10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
\log (P\textsubscript{L}/Pa) = -4579/(T/K) + 13.29 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa-m\textsuperscript{3}/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
113.5 (calculated-P/C, Burkhard 1984)
8.41 (20°C, calculated-P/C, Murphy et al. 1987)
44.95 (calculated-QSPR, Dunnivant et al. 1992)
15.77, 31.39, 60.5, 113.1 ± 0.4, 188.6 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
\ln K_{\text{AW}} = 21.891 - 7457.3/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{\text{AW}} = \exp\left[-(62.0/kJ\cdot mol^{-1}/K^{-1})/R\right] + (0.182/kJ\cdot mol^{-1}/K^{-1})/R\}; where R = 8.314 J\cdot K^{-1}\cdot mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
107.9 (exptl. data, Bamford et al. 2002)
\ln K_{\text{AW}} = -\Delta H_{\text{g}}/RT + \Delta S_{\text{g}}/R; R is the ideal gas constant, \Delta H_{\text{g}} = 62 ± 5 kJ/mol, \Delta S_{\text{g}} = 0.18 ± 0.02 kJ/mol\cdot K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
7.21 (calculated-TSA, Burkhard 1984)
6.78 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
Polychlorinated Biphenyls (PCBs)

6.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (recommended, Sangster 1993)
6.7947 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 10.22 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log $BCF$ or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
- 7.01 (suspended particulate matter, Burkhard 1984)
- 5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 2$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03$ d$^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 21$ d in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.189 2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189)

![Chemical Structure](image)

Common Name: 2,3,3',4,4',5,5'-Heptachlorobiphenyl
Synonym: PCB-189, 2,3,3',4,4',5,5'-heptachloro-1,1'-biphenyl
Chemical Name: 2,3,3',4,4',5,5'-heptachlorobiphenyl
CAS Registry No: 39635-31-9
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323

Melting Point (°C):
- 170 (Burkhard et al. 1985b)
- 163 (Brodsky & Ballschmiter 1988)

Boiling Point (°C):

Density (g/cm³):
- 330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0378 (mp at 170°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
- 0.0063 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- $7.53 \times 10^{-5}$ (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
- $6.26 \times 10^{-5}$ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
- $1.30 \times 10^{-4}$; $4.47 \times 10^{-5}$ (generator column-GC/ECD, estimated, Hong & Qiao 1995)
- $4.05 \times 10^{-4}$ (calculated-mp and $K_{\text{OW}}$, Ran et al. 2002)
- 0.000063 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- $1.44 \times 10^{-4}$ (P_L supercooled liquid GC-RT correlation, Burkhard et al. 1985a)
- $5.95 \times 10^{-5}$ (GC-RI correlation, Burkhard et al. 1985b)
- $4.77 \times 10^{-5}$, $3.30 \times 10^{-5}$ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- $2.69 \times 10^{-5}$ (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)

log (P_L/Pa) = −5300/(T/K) + 13.46 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa-m³/mol at 25°C):
- 9.18 (calculated-P/C, Burkhard et al. 1985a)
- 6.74 (calculated-QSPR, Dunnivant et al. 1992)
- 0.903 (calculated-QSPR, Achman et al. 1993)
- 28.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

$\ln K_{\text{AW}} = -\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R$; R is the ideal gas constant, $\Delta H_{\text{f}} = 149 \pm 13$ kJ/mol, $\Delta S_{\text{f}} = 0.46 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
- 7.14 (calculated-TSA, Burkhard 1984)
- 7.72 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
- 7.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 12.81, 11.54; 11.45 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 11.15 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:
- 6.41, 7.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.94 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.817 (as log $K_a$, association coefficient with marine humic substance, calculated-$\chi$, Sabljic et al. 1989)

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_2 = 0.011$ d$^{-1}$ with $t_{1/2} = 64$ d and $k_2 = 0.012$ d$^{-1}$ with $t_{1/2} = 58$ d for food concn of 19 ng/g and 138 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 176$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: reported biological $t_{1/2} > 200$ d for heptachlorobiphenyls in carp (Niimi 1987)
Depuration $t_{1/2} = 58$–64 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
Depuration $t_{1/2} = 176$ d for high-dose treatment, $t_{1/2} = 171$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.190 2,3,3′,4,4′,5,6-Heptachlorobiphenyl (PCB-190)

Common Name: 2,3,3′,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-190, 2,3,3′,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 41411-64-7
Molecular Formula: C₁₂H₃Cl₇
Molecular Weight: 395.323
Melting Point (°C):
117.0 (Burkhard et al. 1985b)
116 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.125 (mp at 117°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.00767 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.98 × 10⁻⁴ (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
1.98 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
2.20 × 10⁻⁴ (calculated-QSPR, Dunnivant et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.96 × 10⁻⁴ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.70 × 10⁻⁵ (GC-RI correlation, Burkhard et al. 1985b)
1.09 × 10⁻⁴, 1.47 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.13 × 10⁻⁵, 7.08 × 10⁻⁵ (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –5109/(T/K) + 13.17 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
10.06 (calculated-P/C, Burkhard 1984)
11.37 (calculated-QSPR, Dunnivant et al. 1992)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_IW = –ΔH_fus/RT + ΔS_fus/R; R is the ideal gas constant, ΔH_fus = 149 ± 13 kJ/mol, ΔS_fus = 0.46 ± 0.04 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_OW:
7.05 (calculated-TSA, Burkhard 1984)
7.08 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
7.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.08 (recommended, Sangster 1993)
7.2887 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_OA at 25°C or as indicated:
12.09, 10.87 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
10.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Polychlorinated Biphenyls (PCBs)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 6.84 (suspended particulate matter, Burkhard 1984)
- 5.675 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
  - Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
    - $k_1 = 2$ (food lipid (mg)/(g worm lipid-d); $k_2 = 0.03$ d$^{-1}$ (earthworm, Wågman et al. 2001)
    - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
    - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
  - Biota: elimination $t_{1/2} = 25$ d in earthworm given contaminated food (Wågman et al. 2001)
  - depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 184$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.191 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl (PCB-191)

Common Name: 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-191, 2,3,3′,4,4′,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 74472-50-7
Molecular Formula: C_{12}H_3Cl_7
Molecular Weight: 395.323
Melting Point (°C):
126 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
6.60 × 10⁻³ (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14 × 10⁻⁴ (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.98 × 10⁻⁴ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.89 × 10⁻⁴ (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55 × 10⁻⁴, 5.68 × 10⁻⁶ (supercooled liquid P_L, calculated-MW, GC-RI correlation, calculated-MCI \(\chi\), Burkhard et al. 1985b)
1.05 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = −5109/(T/K) + 13.15 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
17.33 (calculated-P/C, Burkhard 1984)
13.48 (calculated-QSAR, Dunnivant et al. 1992)
1.367 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln \(K_{\text{AW}}\) = −\(\Delta H_{\text{f}}/RT + \Delta S_{\text{f}}/R\); R is the ideal gas constant, \(\Delta H_{\text{f}} = 149 \pm 13\) kJ/mol, \(\Delta S_{\text{f}} = 0.46 \pm 0.04\) kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
7.12 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.21 (recommended, Sangster 1993)
7.3254 (calculated-molecular properties MNDO-AMI method, Makino 1998)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\) at 25°C or as indicated:
12.07, 10.91; 10.93 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.10 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

$6.92$ (suspended particulate matter, Burkhard 1984)

$5.659$ (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Half-Lives in the Environment:
7.1.1.192 2,3',4,5,5',6-Heptachlorobiphenyl (PCB-192)

Common Name: 2,3',4,5,5',6-Heptachlorobiphenyl
Synonym: PCB-192, 2,3',4,5,5',6-heptachloro-1,1'-biphenyl
Chemical Name: 2,3',4,5,5',6-heptachlorobiphenyl
CAS Registry No: 74472-51-8
Molecular Formula: C$_{12}$H$_3$Cl$_7$
Molecular Weight: 395.323
Melting Point (°C): 142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta$H$_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta$S$_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta$S$_{\text{fus}}$ = 56 J/mol K), F:
Water Solubility (g/m$^3$ or mg/L at 25°C):
6.92 × 10$^{-3}$ (S$_L$ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14 × 10$^{-4}$ (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
1.57 × 10$^{-4}$ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.89 × 10$^{-4}$ (P$_L$ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55 × 10$^{-4}$, 3.23 × 10$^{-4}$, 2.96 × 10$^{-5}$ (P$_L$, calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985b)
1.75 × 10$^{-4}$, 2.49 × 10$^{-4}$ (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.12 × 10$^{-5}$, 1.41 × 10$^{-3}$ (supercooled liquid P$_L$, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P$_L$/Pa) = –5109/(T/K) + 13.38 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
16.52 (calculated-P/C, Burkhard 1984)
19.40 (calculated-QSPR, Dunnivant et al. 1992)
1.37 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{\text{AW}}$ = $-\Delta$H$_{\text{f}}$/2RT + $\Delta$S$_{\text{f}}$/R; R is the ideal gas constant, $\Delta$H$_{\text{f}}$ = 149 ± 13 kJ/mol, $\Delta$S$_{\text{f}}$ = 0.46 ± 0.04 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
7.09 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k correlation, Brodsky & Ballschmiter 1988)
7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{\text{oa}}$:
10.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_0$:

Sorption Partition Coefficient, log $K_{OC}$:

- 6.89 (suspended particulate matter, Burkhard 1984)
- 5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:
7.1.1.193 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl (PCB-193)

Common Name: 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-193, 2,3,3′,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 69782-91-8
Molecular Formula: C_{12}H_{3}Cl_{7}
Molecular Weight: 395.323
Melting Point (°C): 154 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:

© 2006 by Taylor & Francis Group, LLC
Polychlorinated Biphenyls (PCBs)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated:
- 11.99, 10.82; 10.02 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 10.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log \( K_b \):

Sorption Partition Coefficient, log \( K_{OC} \):
- 6.89 (suspended particulate matter, Burkhard 1984)
- 5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient log \( K_a \), calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):
  \[ k_1 = 5 \text{ (food lipid mg)/(g worm lipid-d); } k_2 = 0.03 \text{ d}^{-1} \text{ (earthworm, Wågman et al. 2001)} \]

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: elimination \( t_{1/2} = 21 \text{ d} \) in earthworm given contaminated food (Wågman et al. 2001)
7.1.1.194 2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl (PCB-194)

**Chemical Name:** 2,2′,3,3′,4,4′,5,5′-octachlorobiphenyl  
**Synonym:** PCB-194, 2,2′,3,3′,4,4′,5,5′-octachloro-1,1′-biphenyl

**CAS Registry No:** 35694-08-7  
**Molecular Formula:** C_{12}H_{2}Cl_{8}  
**Molecular Weight:** 429.768  
**Melting Point (°C):**  
- 159–160 (Binns & Suschitzky 1971)  
- 156 (Kühne et al. 1995; Ruelle & Kesselring 1997)  
**Boiling Point (°C):**  
**Density (g/cm³):** 1.507 (at 22°C)  
**Molar Volume (cm³/mol):**  
- 351.8 (calculated-Le Bas method at normal boiling point)  
- 263.2 (Ruelle & Kesselring 1997)  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**  
**Entropy of Fusion, ΔS_{fus} (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.0484 (mp at 159°C)  
0.0474 (Mackay et al. 1980; Shiu & Mackay 1986)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):**  
- 0.0072 (shake flask-GC/ECD, Wallnöfer et al. 1973)  
- 0.000272 (generator column-GC/ECD, Weil et al. 1974)  
- 8.58 × 10⁻⁵ (RP-HPLC-K’ correlation, Brodsky & Ballschmiter 1988)  
- 0.00124 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)  
- 3.79 × 10⁻³; 2.40 × 10⁻³ (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)  
log S_{L}/(mol m⁻³) = −1533/(T/K) − 0.11 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
- 2.03 × 10⁻⁵ (GC-RI correlation, Burkhard et al. 1985a)  
- 3.86 × 10⁻⁴ (supercooled liquid P_{L}, GC-RI correlation, Burkhard et al. 1985b)  
- 2.07 × 10⁻⁵; 1.79 × 10⁻⁵ (supercooled liquid P_{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)  
1.29 × 10⁻⁵ (supercooled liquid P_{L}, GC-RI correlation, Fischer et al. 1992)  
log (P_{L}/Pa) = −5402/(T/K) + 13.43 (GC-RT correlation, Falconer & Bidleman 1994)  
2.04 × 10⁻⁵; 2.45 × 10⁻⁵ (supercooled liquid P_{L}; LDV literature derived value, FAV final adjusted value, Li et al. 2003)  
log P_{L}/Pa = −5099/(T/K) + 12.49 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)  
**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):**  
- 47.52 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)  
- 10.13 (wetted-wall column-GC, Brunner et al. 1990)  
- 6.79 (calculated-QSPR, Dunnivant et al. 1992)  
- 1.01 (calculated-QSPR, Achman et al. 1993)  
- 0.34 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)  
- 10.9 (from 11°C expltl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_m/RT + \Delta S_m/R$; $R$ is the ideal gas constant, $\Delta H_m = 169 \pm 6$ kJ/mol, $\Delta S_m = 0.52 \pm 0.02$ kJ/mol·K
(Bamford et al. 2002)—see Comment by Goss et al. 2004
6.76, 4.37 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log $[H/(Pa \text{ m}^3/\text{mol})] = -3566/(T/K) + 12.60$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log $K_{ow}$:
8.68 (RP-TLC-RT correlation, Bruggeman et al. 1982)
9.35 (HPLC-RT correlation, Shaw & Connell 1982)
7.62 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
7.67 (generator column-GC, Hawker & Connell 1988a)
6.94 (generator column-GC, Larsen et al. 1992)
7.65 (recommended, Sangster 1993)
7.67, 7.80, 9.35 (quoted lit. values, Hansch et al. 1995)
7.67, 7.76 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated and reported temperature dependence equations:
10.50 (calculated-$K_{ow}/K_{aw}$, Wania & Mackay 1996)
12.83, 11.59; 11.71 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
11.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
11.31, 11.13 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log $K_{oa} = 4906/(T/K) - 5.33$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log $BCF$ at 25°C or as indicated:
5.81 (guppy, 3.5% lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
4.35 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
4.18 (worms, Oliver 1987c)
4.35 (guppy, calculated-$C_p/C_w$ or $k_1/k_2$, Connell & Hawker 1988; Hawker 1990)
4.81 (guppy, estimated, Banerjee & Baughman 1991)
5.81; 7.34 (22°C, zebrafish: log $BCF_w$ wet wt basis; log $BCF_l$ lipid wt basis, Fox et al. 1994)
5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{oc}$:
7.27 (suspended particulate matter, calculated-$K_{ow}$, Burkhard 1984)
6.5–7.1, 6.8; 7.80 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_m$, Lara & Ernst 1989)
5.943, 6.016 (marine humic substances or 5 mg/L DOC, quoted; calculated-MCI $\chi$, reported as log $K_m$, Sabljic et al. 1989)
6.41, 6.20, 6.06 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.96 (soil, calculated-Characteristic Root Index CRI model, Saçan & Balcioğlu 1996)
7.30 (soil, calculated-$K_{ow}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:
Volatileization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 > 0.0007$ d⁻¹ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 150$ d⁻¹; $k_2 = 0.007$ d⁻¹ (guppy, Bruggeman et al. 1984)
$k_1 = 1000$ d⁻¹ (guppy, Opperhuizen 1986)
log $k_1 = 2.18$ d$^{-1}$; log $1/k_2 = 2.15$ d (fish, quoted, Connell & Hawker 1988)

$k_1 = 5640$ d$^{-1}$; $k_2 = 0.00865$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 174$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:

Biota: $t_{1/2} > 1000$ d in rainbow trout and $t_{1/2} = 78$ d in its muscle (Niimi & Oliver 1983);

$t_{1/2} = 100$ d in guppy (Bruggeman et al. 1984);

$t_{1/2} = 220$ d in worms at 8°C (Oliver 1987c).

Depuration $t_{1/2} = 158$ d for high-dose treatment, $t_{1/2} = 174$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.195 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl (PCB-195)

Common Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
Synonym: PCB-195, 2,2′,3,3′,4,4′,5,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
CAS Registry No: 52663-78-2
Molecular Formula: C_{12}H_{2}Cl_{8}
Molecular Weight: 429.768
Melting Point (°C): 176 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00334 (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
2.204 × 10⁻⁵ (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81 × 10⁻⁵ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.92 × 10⁻⁵ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.12 × 10⁻⁴ (GC-RJ correlation, Burkhard et al. 1985b)
4.53 × 10⁻⁵, 7.46 × 10⁻⁵ (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.19 × 10⁻⁵, 3.63 × 10⁻⁵ (supercooled liquid Pₗ, GC-RJ correlation, different stationary phases, Fischer et al. 1992)
log (Pₗ/Pa) = –5244/(T/K) + 13.24 (GC-RJ correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
12.77 (calculated-P/C, Burkhard 1984)
1.115 (wetted-wall column-GC/ECD, Brunner et al. 1990)
12.01 (calculated-QSPR, Dunnivant et al. 1992)
14.13 ± 0.78 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
0.079, 0.485, 2.724, 14.13, 54.5 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 62.305 – 20086.6/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = \exp[-(167.0/kJ·mol⁻¹)/RT] + (0.518/kJ·mol⁻¹·K⁻¹)/R]; where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
15.1 (exptl. data, Bamford et al. 2002)
ln K_{AW} = –ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 167 ± 13 kJ/mol, ΔS_{f} = 0.52 ± 0.05 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
7.49 (calculated-TSA, Burkhard 1984)
7.35 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.56 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 11.13, 10.04; 10.02 (0, 20°C, GC-k correlation; calculated at 20°C, Zhang et al. 1999)
- 11.26 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:
- 5.92; 7.45 (zebrafish: log BCF$_W$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log $K_{OC}$:
- 7.29 (suspended particulate matter, Burkhard 1984)
- 5.78, 5.59, 5.55, 5.32 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_a$, Lara & Ernst 1989)
- 5.78; 5.87 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_a$, observed; calculated-MCI $\chi$, Sabljic et al. 1989)
- 6.42, 6.26, 6.14 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_1 = 5930$ d$^{-1}$; $k_2 = 0.00711$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
  - $k_2 = 0.011$ d$^{-1}$ with $t_{1/2} = 67$ d and $k_2 = 0.011$ d$^{-1}$ with $t_{1/2} = 61$ d for food concn of 24 ng/g and 126 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
  - $k_3 = 0.005$ d$^{-1}$ with $t_{1/2} = 143$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)
  - $k_3 = 0.004$ d$^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYP1A-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 61$–67 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
  - depuration $t_{1/2} = 143$ d for high-dose treatment, $t_{1/2} = 158$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.196 2,2',3,3',4,4',5,6'-Octachlorobiphenyl (PCB-196)

Common Name: 2,2',3,3',4,4',5,6'-Octachlorobiphenyl
Synonym: PCB-196, 2,2',3,3',4,4',5,6'-octachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',4,4',5,6'-Octachlorobiphenyl
CAS Registry No: 42740-50-1
Molecular Formula: C₁₂H₂Cl₈
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₜ (kJ/mol):
Entropy of Fusion, ΔSₘₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₜ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
2.91 × 10⁻³ (Sₗ, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.63 × 10⁻⁴ (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
6.81 × 10⁻⁵ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.87 × 10⁻⁴ (Pₗ, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.40 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
6.11 × 10⁻⁵, 8.41 × 10⁻⁵ (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47 × 10⁻⁵, 5.89 × 10⁻⁵ (supercooled liquid Pₗ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₗ/Pa) = –5244/(T/K) + 13.37 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
71.94 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
13.23 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₘₚ = –ΔHₘ/R + ΔSₘ/R; R is the ideal gas constant, ΔHₘ = 167 ± 13 kJ/mol, ΔSₘ = 0.52 ± 0.05 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log Kₐ(w):
7.57 (calculated-TSA, Burkhard 1984)
7.43 (RP-HPLC-k' correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.43 (recommended, Sangster 1993)
7.70 (estimated, Girvin & Scott 1997)
7.4190 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 12.27, 11.03; 11.19 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 11.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{oc}$:
- 7.37 (suspended particulate matter, Burkhard 1984)
- 5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 7.30 (soil-organic carbon, calculated-$K_{OW}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 168$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
  - $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration exp.- high-dose treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 156$ d for high-dose treatment, $t_{1/2} = 168$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.197 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl (PCB-197)

Common Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
Synonym: PCB-197, 2,2′,3,3′,4,4′,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
CAS Registry No: 33091-17-7
Molecular Formula: C_{12}H_{2}Cl_{8}
Molecular Weight: 429.768
Melting Point (°C):
132  (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm³):
351.8  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0892 (mp at 132°C)

Water Solubility (g/m³ or mg/L at 25°C):
\[2.81 \times 10^{-3} \text{ (S\textsubscript{l} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)}\]
\[3.41 \times 10^{-4} \text{ (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)}\]
\[1.71 \times 10^{-4} \text{ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)}\]
\[1.03 \times 10^{-4} \text{ (calculated-QSPR, Dunnivant et al. 1992)}\]

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\[\begin{align*}
6.79 \times 10^{-4} & \text{ (P\textsubscript{l} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)} \\
5.93 \times 10^{-5} & \text{ (GC-RI correlation, Burkhard et al. 1985b)} \\
1.90 \times 10^{-4}, 1.22 \times 10^{-4} & \text{ (supercooled liquid P\textsubscript{l}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)} \\
9.12 \times 10^{-5} & \text{ (supercooled liquid P\textsubscript{l}, GC-RI correlation, Fischer et al. 1992)} \\
\end{align*}\]
\[
\log (P\textsubscript{l}/P\textsubscript{a}) = -4581/(T/K) + 12.52 \text{ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)}
\]

Henry’s Law Constant (Pa·m³/mol at 25°C):
\[94.03 \text{ (calculated-P/C, Burkhard 1984)}\]
\[25.69 \text{ (calculated-QSPR, Dunnivant et al. 1992)}\]
\[97.5 \text{ (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)}\]
\[
\ln K_{AW} = -\Delta H_{f}/RT + \Delta S_{f}/R; R \text{ is the ideal gas constant, } \Delta H_{f} = 145 \pm 7 \text{ kJ/mol, } \Delta S_{f} = 0.46 \pm 0.04 \text{ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004)}
\]

Octanol/Water Partition Coefficient, log $K_{ow}$:
\[7.59 \text{ (calculated-TSA, Burkhard 1984)}\]
\[7.21 \text{ (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)}\]
\[7.30 \text{ (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)}\]
\[7.21 \text{ (recommended, Sangster 1993)}\]

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:
\[\begin{align*}
11.74, 10.52; 10.68 & \text{ (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)} \\
11.30 & \text{ (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)} \\
\end{align*}\]
Bioconcentration Factor, log BCF or log $K_{bi}$:

Sorption Partition Coefficient, log $K_{OC}$:

- 7.39 (suspended particulate matter, Burkhard 1984)
- 5.699 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
7.1.1.198 2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB-198)

Common Name: 2,2',3,3',4,5,5',6-Octachlorobiphenyl
Synonym: PCB-198, 2,2',3,3',4,5,5',6-octachloro-1,1'-biphenyl
Chemical Name: 2,2',3,3',4,5,5',6-Octachlorobiphenyl
CAS Registry No: 68194-17-2
Molecular Formula: C_{12}H_{2}Cl_{8}
Molecular Weight: 429.768
Melting Point (°C): 162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
- 3.03 × 10⁻³ (S₂, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
- 1.63 × 10⁻⁴ (RP-HPLC-k’ correlation, Brodsky & Ballischmier 1988)
- 8.58 × 10⁻⁵ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
- 1.48 × 10⁻⁴ (P₁, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
- 3.44 × 10⁻⁴, 1.67 × 10⁻⁴, 5.68 × 10⁻⁶ (GC-RI correlation, Burkhard et al. 1985b)
- 6.85 × 10⁻⁵, 1.224 × 10⁻⁴ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 5.01 × 10⁻⁵, 7.08 × 10⁻⁵ (supercooled liquid P₁, GC-RI correlation, different stationary phases, Fischer et al. 1992)
  log (P₁/P₀) = −5244/(T/K) + 13.42 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 20.97 (calculated-P/C, Burkhard 1984)
- 1.419 (wetted wall column-GC/ECD, Brunner et al. 1990)
- 15.62 (calculated-QSPR, Dunnivant et al. 1992)
- 15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
  ln $K_{\text{AW}} = −\Delta H_{\text{fus}}/RT + \Delta S_{\text{fus}}/R$; R is the ideal gas constant, $\Delta H_{\text{fus}} = 167 ± 13$ kJ/mol, $\Delta S_{\text{fus}} = 0.52 ± 0.05$ kJ/mol-K
  (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
- 7.55 (calculated-TSA, Burkhard 1984)
- 7.43 (RP-HPLC-k’ correlation, Brodsky & Ballischmier 1988)
- 7.43 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{\text{OA}}$ at 25°C or as indicated:
- 12.32, 11.05; 10.02 (0, 20°C, multi-column GC-k’ correlation; calculated at 20°C, Zhang et al. 1999)
- 11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_{\text{B}}$:
Sorption Partition Coefficient, log $K_{oc}$:
- 7.35 (suspended particulate matter, Burkhard 1984)
- 5.91, 5.63, 5.56, 5.23 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_{ah}$, Lara & Ernst 1989)
- 5.91; 5.86 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{ah}$, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004$ d$^{-1}$ with $t_{1/2} = 185$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 158$ d for high-dose treatment, $t_{1/2} = 185$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.199 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl (PCB-199)

Common Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
Synonym: PCB-199, 2,2′,3,3′,4,5,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
CAS Registry No: 52663-75-9
Molecular Formula: C\textsubscript{12}H\textsubscript{2}Cl\textsubscript{8}
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):
Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS\textsubscript{fus} = 56 J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
3.23 × 10\textsuperscript{-3} (S\textsubscript{L} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.41 × 10\textsuperscript{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.41 × 10\textsuperscript{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.20 × 10\textsuperscript{-4} (P\textsubscript{L} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.57 × 10\textsuperscript{-4} (GC-RI correlation, Burkhard et al. 1985b)
9.35 × 10\textsuperscript{-5}, 1.67 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.05 × 10\textsuperscript{-4}, 2.04 × 10\textsuperscript{-4} (supercooled liquid P\textsubscript{L}: GC-RI correlation, different stationary phases, reported as the revised order PCB-200-2,2′,3,3′,4,5,6,6′-PCB-200: 2,2′,3,3′,4,5,6,6′-PCB-200: Fischer et al. 1992)
log (P\textsubscript{L}/Pa) = –5244/(T/K) + 13.36 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
42.66 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
23.0 (calculated-QSPR, Dunnivant et al. 1992)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K\textsubscript{AW} = –ΔH\textsubscript{H}/RT + ΔS\textsubscript{H}/R; R is the ideal gas constant, ΔH\textsubscript{H} = 167 ± 13 kJ/mol, ΔS\textsubscript{H} = 0.52 ± 0.05 kJ/mol K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K\textsubscript{OW}:
7.51 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.28 (quoted lit., Maruya & Lee 1998-reported as revised order PCB-200: 2,2′,3,3′,4,5,6,6′-PCB)
7.21 (revised previously quoted value; Maruya & Lee 2000)
Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:
12.28, 11.05; 10.02 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
11.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Biota Sediment Accumulation Factor, BSAF:
96 (trout in Lake Ontario, Niimi 1996)
0.26, 7.1, 1.1 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, $\log K_{OC}$:
7.31 (suspended particulate matter, Burkhard 1984)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_a$, Lara & Ernst 1989)
5.711 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.44, 6.18, 6.02 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
7.1.1.200 2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200)

**Chemical Name:** 2,2',3,3',4,5,6,6'-Octachlorobiphenyl

**Synonym:** PCB-200, 2,2',3,3',4,5,6,6'-octachloro-1,1'-biphenyl

**CAS Registry No:** 52663-73-7

**Molecular Formula:** C_{12}H_{2}Cl_{8}

**Molecular Weight:** 429.768

**Melting Point (°C):**
130 (estimated, Abramowitz & Yalkowsky 1990)

**Boiling Point (°C):**

**Density (g/cm³):**
351.8 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:**

**Water Solubility (g/m³ or mg/L at 25°C):**
2.93 × 10^{-3} (S_{l} supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.105 × 10^{-3}, 1.79 × 10^{-4}, 1.08 × 10^{-4}, 2.01 × 10^{-4} (RP-HPLC-k' correlation, different and mobile stationary phases, Brodsky & Ballschmiter 1988)
4.30 × 10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
4.56 × 10^{-4} (P_{l} supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.37 × 10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.75 × 10^{-4}, 3.32 × 10^{-4} (supercooled liquid P_{l}, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.89 × 10^{-5}, 5.89 × 10^{-5} (supercooled liquid P_{l}, GC-RI correlation, different stationary phases, reported in revised order as PCB-201-2,2',3,3',4,4',6,6'-, Fischer et al. 1992)

log (P_{l}/Pa) = −4851/(T/K) + 12.24 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
2.34 × 10^{-5} (P_{l}, calculated-MCI χ and Characteristic Root Index CRI, Şaçan & Balcioğlu 1998)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**
66.98 (calculated-P/C, Burkhard 1984)
1.50 (calculated-QSPR, Achman et al. 1993)
24.36 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 145 ± 7 kJ/mol, ΔS_{f} = 0.46 ± 0.04 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

**Octanol/Water Partition Coefficient, log K_{OW}:**
7.57 (calculated-TSA, Burkhard 1984)
7.16, 7.54, 7.16, 7.36; 7.35 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.35 (recommended, Sangster 1993)
7.27 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
   12.05, 10.82 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
   11.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
   7.36 (suspended particulate matter, Burkhard 1984)
   5.50, 5.72, 5.68, 5.36 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log $K_h$, Lara & Ernst 1989)
   5.68; 5.70 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_h$, observed; calculated-MCI $\chi$, Sabljic et al. 1989)
   7.05 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcıoğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
7.1.1.201 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl (PCB-201)

Common Name: 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl
Synonym: PCB-201, 2,2′,3,3′,4,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl
CAS Registry No: 40186-71-8
Molecular Formula: C₁₂H₂Cl₈
Molecular Weight: 429.768
Melting Point (°C):
    162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³): 351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘ (kJ/mol):
Entropy of Fusion, ΔSₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
    3.06 × 10⁻³ (S₁ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
    2.204 × 10⁻⁴ (RP-HPLC-K’ correlation, Brodsky & Ballschmiter 1988)
    8.58 × 10⁻⁵ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    4.56 × 10⁻¹ (P₁ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
    5.06 × 10⁻¹ (GC-RI correlation, Burkhard et al. 1985b)
    5.94 × 10⁻², 1.0 × 10⁻¹ (supercooled liquid P₁, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
    1.41 × 10⁻¹ (supercooled liquid P₁, GC-RI correlation, different stationary phases, reported as revised order PCB-199, 2,2′,3,3′,4,5′,6′-octachlorobiphenyl, Fischer et al. 1992)
    log (P₁/Pa) = –4581/(T/K) + 12.51 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
    64.54 (calculated-P/C, Burkhard 1984)
    1.72 (wetted wall column-GC/ECD, Brunner et al. 1990)
    13.23 (calculated-QSPR, Dunnivant et al. 1992)
    0.990 (calculated-QSPR, Achman et al. 1993)
    0.156, 0.457 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
    95.8 ± 4.4 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
    1.069, 5.14, 22.98, 95.8, 308 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
    K₆₈W = exp−[−(144.5/kJ·mol⁻¹)/RT] + (0.458/kJ·mol⁻¹·K⁻¹)R]; where R = 8.314 J·K⁻¹·mol⁻¹ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
    97.5 (exptl. data, Bamford et al. 2002)
    ln K₆₈W = −ΔH/RT + ΔS/R; R is the ideal gas constant, ΔH = 145 ± 7 kJ/mol, ΔS = 0.46 ± 0.03 kJ/mol·K
    (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K₁₈W:
    7.54 (calculated-TSA, Burkhard 1984)
    7.35 (RP-HPLC-k’ correlation, Brodsky & Ballschmiter 1988)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

- 12.22, 10.98 (0, 20°C, multi-column GC-$k’$ correlation, Zhang et al. 1999)
- 11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_B$:

- 5.88; 7.41 (zebrafish: log BCF$_W$ wet wt basis; log BCF$_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log $K_{OC}$:

- 7.34 (suspended particulate matter, Burkhard 1984)
- 5.913; 5.857 (marine humic substances with 5 mg/L DOC, reported as association coefficient log $K_{so}$, observed; calculated-MCI $1^\chi$, Sabljic et al. 1989)
- 6.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 7.30 (soil, estimated-log $K_{org}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_1 = 5950$ d$^{-1}$; $k_2 = 0.00776$ d$^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- $k_1 = 0.005$ d$^{-1}$ with $t_\frac{1}{2} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_1 = 0.004$ d$^{-1}$ with $t_\frac{1}{2} = 172$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:

Biota: depuration $t_\frac{1}{2} = 153$ d for high-dose treatment, $t_\frac{1}{2} = 172$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.202 2,2’,3,3’,5,5’,6,6’-Octachlorobiphenyl (PCB-202)

Common Name: 2,2’,3,3’,5,5’,6,6’-Octachlorobiphenyl
Synonym: PCB-202, 2,2’,3,3’,5,5’,6,6’-octachloro-1,1’-biphenyl
Chemical Name: 2,2’,3,3’,5,5’,6,6’-Octachlorobiphenyl
CAS Registry No: 2136-99-4
Molecular Formula: C$_{12}$H$_{2}$Cl$_{8}$
Molecular Weight: 429.768
Melting Point (°C):
161 (Van Roosmalen 1934; Burkhard et al. 1985a; Erickson 1986; Lide 2003)
Boiling Point (°C):
Density (g/cm$^3$ at 20°C): 1.507
Molar Volume (cm$^3$/mol):
351.8 (calculated-Le Bas method at normal boiling point)
263.2 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, $\Delta$H$_{fus}$ (kJ/mol):
22.80 (Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, $\Delta$S$_{fus}$ (J/mol K):
52.72 (Miller et al. 1984; Shiu & Mackay 1986; selected, Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming $\Delta$S$_{fus}$ = 56 J/mol K), F:
0.0463 (mp at 161°C)
0.0443 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.80 × 10$^{-4}$ (generator column-GC/ECD, Weil et al. 1974;)
3.93 × 10$^{-4}$ (generator column-GC/ECD, Miller et al. 1984,1985)
1.47 × 10$^{-4}$ (generator column-GC/ECD, measured range 20–50°C, Dickhut et al. 1986)
1.14 × 10$^{-4}$, 1.47 × 10$^{-4}$, 2.12 × 10$^{-4}$, 4.66 × 10$^{-4}$ (4. 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)

$\ln x = -6098/(T/K) – 5.333$, temp range 4–32°C, $\Delta$H$_{diss}$ = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -2652/(T/K) – 2.308$, $\Delta$H$_{diss}$ = 50.6 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 6.91 \times 10^{-11} \exp(0.064\cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

2.53 × 10$^{-4}$, 5.93 × 10$^{-4}$, 6.51 × 10$^{-4}$, 2.36 × 10$^{-4}$ (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

$\ln x = -5.34 – 6100/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.90 × 10$^{-3}$ (extrapolated gas saturation-GC, measured range 29–61.2°C, Burkhard et al. 1984)

log (P/Pa) = 13.262 – 5307.3/(T/K); temp range 29–61.2°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)

2.89 × 10$^{-3}$, 6.43 × 10$^{-4}$ (solid P$_s$, P$_s$ calculated from P$_u$ using fugacity ratio F, Burkhard et al. 1985a)

5.40 × 10$^{-4}$ (supercooled liquid P$_L$, GC-RI correlation, Burkhard et al. 1985b)

1.70 × 10$^{-4}$, 3.91 × 10$^{-4}$ (supercooled liquid P$_L$, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

6.59 × 10$^{-4}$, 5.26 × 10$^{-4}$ (supercooled P$_L$, converted from literature P$_s$ with different $\Delta$S$_{fus}$ values, Hinckley et al. 1990)

2.22 × 10$^{-4}$ (P$_{GC}$ by GC-RT correlation with $p,p'$-DDT as reference standard, Hinckley et al. 1990)
log \( \frac{P}{\text{Pa}} = 12.99 - 4851/(T/K) \) (GC-RT correlation, Hinckley et al. 1990)

\( 2.40 \times 10^{-4} \) (supercooled liquid \( P_L \); GC-RI correlation, Fischer et al. 1992)

\( \log (P/\text{Pa}) = -4851/(T/K) + 12.99 \) (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

\( (2.41 - 29.5) \times 10^{-6} \); \( (1.73 - 5.40) \times 10^{-4} \) (literature solid \( P_s \) range; literature liquid \( P_L \) range, Delle Site 1997)

\( \log (P/\text{Pa}) = 13.282 - 5307.3/(T/K); \) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C):

- 75.79 (calculated-P/C, Burkhard et al. 1985b)
- 38.08 (calculated-P/C, Shiu & Mackay 1986)
- 1.82 (wetted-wall column-GC, Brunner et al. 1990)
- 22.63 (calculated-QSPR, Dunnivant et al. 1992)
- 1.50 (calculated-QSPR, Achman et al. 1993)
- 97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

\( \ln K_{AW} = -\Delta H_f/RT + \Delta S_m/R; \) R is the ideal gas constant, \( \Delta H_f = 145 \pm 7 \text{ kJ/mol}, \Delta S_m = 0.46 \pm 0.03 \text{ kJ/mol·K} \)

(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

- 9.77 (Hansch & Leo 1979)
- 8.42 (TLC-RT correlation, Bruggeman et al. 1982)
- 7.11 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 7.14 (generator column-HPLC, Woodburn et al. 1984)
- 7.12 (generator column-GC/ECD, Doucette & Andren 1987,1988)
- 7.01, 7.35, 6.98, 7.31 (RP-HPLC-\( k' \) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 7.21 (generator column-GC, Hawker & Connell 1988a)
- 7.67 (HPLC-RT correlation, Hawker & Connell 1988)
- 7.729 ± 0.031 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 7.54 (HPLC-\( k' \) correlation, Noegrohati & Hammers 1992)
- 7.15 (recommended, Sangster 1993)
- 7.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:

- 11.57, 10.38 (0, 20°C, multi-column GC-\( k' \) correlation; calculated at 20°C, Zhang et al. 1999)
- 10.77 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \):

- 5.82; 7.35 (22°C, zebrafish: log \( BCF_w \) wet wt basis; log \( BCF_L \) lipid wt basis, Fox et al. 1994)
- 5.82, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, \( \log K_{OC} \):

- 7.34 (suspended particulate matter, calculated-\( K_{OW} \), Burkhard 1984)
- 5.61, 5.46, 5.41, 4.99 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient \( \log K_{OC} \), Lara & Ernst 1989)
- 5.610, 5.699 (marine humic substances with 5 mg/L of DOC, reported as association coefficient \( \log K_{OC} \), observed; calculated-MCI \( \chi \), Sabljic et al. 1989)
- 6.36, 6.13, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 7.04 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
- Biodegradation:
- Biotransformation:
Polychlorinated Biphenyls (PCBs)

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

- $k_1 = 5070 \text{ d}^{-1}$; $k_2 = 0.0077 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- $k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 119 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 145 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: depuration $t_{1/2} = 110 \text{ d}$ for high-dose treatment, $t_{1/2} = 145 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

### TABLE 7.1.1.202.1

Reported aqueous solubilities and vapor pressures of 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202) at various temperatures and the reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dickhut et al. 1986</td>
<td>Burkhard et al. 1984</td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>20</td>
<td>$1.29 \times 10^{-4}$</td>
</tr>
<tr>
<td>25</td>
<td>$1.29 \times 10^{-4}$</td>
</tr>
<tr>
<td>32</td>
<td>$2.15 \times 10^{-4}$</td>
</tr>
<tr>
<td>50</td>
<td>$7.73 \times 10^{-4}$</td>
</tr>
<tr>
<td>25.0</td>
<td>$2.90 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

\[ \ln x = A - \frac{B}{(T/K)} \]

\[ \log (P/Pa) = A - \frac{B}{(T/K)} \]

\[ A = -5.333 \]

\[ B = 6098.15 \]

\[ \Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = 50.7 \pm 3.8 \text{ for } 25\text{–}50°C \]

\[ \Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 101.7 \]

© 2006 by Taylor & Francis Group, LLC
FIGURE 7.1.1.202.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202).
7.1.1.203 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl (PCB-203)

Common Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
Synonym: PCB-203, 2,2′,3,4,4′,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
CAS Registry No: 52663-76-0
Molecular Formula: C₁₂H₂Cl₈
Molecular Weight: 429.768
Melting Point (°C): 170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
2.91 × 10⁻³ (Sₗ supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.36 × 10⁻⁴ (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81 × 10⁻⁵ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
1.35 × 10⁻⁴ (Pₗ supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.52 × 10⁻⁴ (GC-RI correlation, Burkhard et al. 1985b)
9.29 × 10⁻⁵, 1.047 × 10⁻⁴ (supercooled liquid Pₗ, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47 × 10⁻³, 5.62 × 10⁻³ (supercooled liquid Pₗ, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (Pₗ/Pa) = –5244/(T/K) + 13.39 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.252 (calculated-P/C, Burkhard 1984)
14.21 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln Kₐₙₜ = –ΔHᵢₚ/RT + ΔSᵢₚ/R; R is the ideal gas constant, ΔHᵢₚ = 167 ± 13 kJ/mol, ΔSᵢₚ = 0.52 ± 0.05 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log Kₒₜₜₜₗ:
7.57 (calculated-TSA, Burkhard 1984)
7.49 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.93 (generator column-GC, Larsen et al. 1992)
7.21 (recommended, Sangster 1993)
7.4825 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
12.36, 11.10 (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log $K_b$:

Sorption Partition Coefficient, log $K_{OC}$:
7.37 (suspended particulate matter, Burkhard 1984)
5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
7.1.1.204  2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl (PCB-204)

Common Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
Synonym: PCB-204, 2,2′,3,4,4′,5,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
CAS Registry No: 74472-52-9
Molecular Formula: C₁₂H₂Cl₈
Molecular Weight: 429.768
Melting Point (°C): 132  (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  351.8  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  2.81 × 10⁻³  (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
  1.49 × 10⁻⁴, 9.85 × 10⁻⁴, 1.83 × 10⁻⁴, 1.49 × 10⁻⁴ (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  4.30 × 10⁻⁴  (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  3.49 × 10⁻⁴  (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
  3.88 × 10⁻⁴  (GC-RI correlation, Burkhard et al. 1985b)
  1.54 × 10⁻⁴, 2.76 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
  1.38 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = –4851/(T/K) + 12.46 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  53.3  (calculated-P/C, Burkhard 1984)
  34.89  (calculated-QSAR, Dunnivant et al. 1992)
  97.5  (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = –ΔH_{H}/RT + ΔS_{H}/R; R is the ideal gas constant, ΔH_{H} = 145 ± 7 kJ/mol, ΔS_{H} = 0.46 ± 0.04 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
  7.59  (calculated-TSA, Burkhard 1984)
  7.46, 7.63, 7.37, 7.45 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
  7.30  (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
  7.48  (recommended, Sangster 1993)
  7.2632  (calculated-molecular properties MNDO-AM1 method, Makino 1998)
Octanol/Air Partition Coefficient, log K_{oa} at 25°C:
  11.15  (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:
- 7.39 (suspended particulate matter, Burkhard 1984)
- 5.699 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
Polychlorinated Biphenyls (PCBs)

7.1.1.205 2,3’,4’,4’,5’,5’,6-Octachlorobiphenyl (PCB-205)

Common Name: 2,3’,4’,4’,5’,5’,6-Octachlorobiphenyl
Synonym: PCB-205, 2,3’,4’,4’,5’,5’,6-octachloro-1,1’-biphenyl
Chemical Name: 2,3’,4’,4’,5’,5’,6-Octachlorobiphenyl
CAS Registry No: 74472-53-0
Molecular Formula: C_{12}H_{2}Cl_{8}
Molecular Weight: 429.768
Melting Point (°C):
150 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point (°C):

Density (g/cm³):
351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
3.50 \times 10^{-3} \text{ (S}_L \text{, supercooled liquid, calculated-TSA, Burkhard et al. 1985a)}
8.58 \times 10^{-5} \text{ (RP-HPLC-}k’\text{ correlation, Brodsky & Ballschmiter 1988)}
3.41 \times 10^{-3} \text{ (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)}

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.84 \times 10^{-5} \text{ (P}_L \text{, supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)}
4.40 \times 10^{-5} \text{ (GC-RI correlation, Burkhard et al. 1985b)}
2.49 \times 10^{-5}, 2.91 \times 10^{-5} \text{ (supercooled liquid P}_L, \text{ GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)}
\log (P_L/Pa) = -5402/(T/K) + 13.51 \text{ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)}

Henry’s Law Constant (Pa·m³/mol at 25°C):
4.70 \text{ (calculated-P/C, Burkhard 1984)}
8.644 \text{ (calculated-QSPR, Dunnivant et al. 1992)}
10.9 \text{ (predicted based on homolig group and ortho-Cl, Bamford et al. 2002)}
\ln K_{\text{AW}} = -\Delta H_{\text{fus}}/R \Delta S_{\text{fus}}/R; R \text{ is the ideal gas constant, } \Delta H_{\text{fus}} = 169 \pm 6 \text{ kJ/mol, } \Delta S_{\text{fus}} = 0.52 \pm 0.05 \text{ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004)}

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
7.47 \text{ (calculated-TSA, Burkhard 1984)}
7.62 \text{ (RP-HPLC-}k’\text{ correlation, Brodsky & Ballschmiter 1988)}
8.00 \text{ (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)}
7.62 \text{ (recommended, Sangster 1993)}
7.7326 \text{ (calculated-molecular properties MNDO-AM1 method, Makino 1998)}

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \) at 25°C or as indicated:
12.86, 11.62 \text{ (0, 20°C, multi-column GC-}k’\text{ correlation, Zhang et al. 1999)}
11.34 \text{ (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)}

Bioconcentration Factor, log BCF or log \( K_{\text{B}} \):
Sorption Partition Coefficient, log $K_{OC}$:

- 7.27 (suspended particulate matter, Burkhard 1984)
- 6.016 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated with molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_\frac{1}{2} = 166 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration, high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_\frac{1}{2} = 168 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration, high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil:

Biota: depuration $t_\frac{1}{2} = 166 \text{ d}$ for high-dose treatment, $t_\frac{1}{2} = 168 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.206 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB-206)

**Chemical Name:** 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl

**Synonym:** PCB-206, 2,2',3,3',4,4',5,5',6-nonochloro-1,1'-biphenyl

**CAS Registry No:** 40186-72-9

**Molecular Formula:** C\textsubscript{12}H\textsubscript{10}Cl\textsubscript{9}

**Molar Volume (cm\textsuperscript{3}/mol):**
- 297.7 (calculated-Le Bas method at normal boiling point)
- 276.1 (Ruelle & Kesselring 1997)

**Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):**
- 28.70 (Opperhuizen et al. 1988; Ruelle et al. 1993)

**Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):**
- 0.016 (Mackay et al. 1980; Shiu & Mackay 1986)

**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations):**
- 0.000112 (generator column-GC/ECD, Weil et al. 1974)
- 2.55 × 10\textsuperscript{-5} (generator column-GC/ECD, measured range 25–50°C, Dickhut et al. 1986)
- 2.55 × 10\textsuperscript{-3}, 5.117 × 10\textsuperscript{-5}, 6.59 × 10\textsuperscript{-5}, 1.32 × 10\textsuperscript{-4} (25, 32, 40, 50°C, generator column-GC/ECD, Dickhut et al. 1986)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
- 1.88 × 10\textsuperscript{-6} (GC-RI correlation, Burkhard et al. 1985a)
- 1.034 × 10\textsuperscript{-4} (supercooled liquid \(P_{L}\), GC-RI correlation, Burkhard et al. 1985b)
- 1.08 × 10\textsuperscript{-5}, 1.53 × 10\textsuperscript{-5} (supercooled liquid \(P_{L}\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

**Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):**
- 27.66 (calculated-P/C, Burkhard et al. 1985b)
- 8.845 (calculated-QSPR, Dunnivant et al. 1992)
- 0.474 (calculated-QSPR, Achman et al. 1993)
15.1 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
\[ \ln K_{AW} = -\Delta H_p/RT + \Delta S_p/R; \]  
\( R \) is the ideal gas constant, \( \Delta H_p = 167 \pm 13 \text{ kJ/mol}, \Delta S_p = 0.52 \pm 0.05 \text{ kJ/mol-K} \)  
(Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 9.14 (RP-TLC-\( k' \) correlation, Bruggeman et al. 1982)
- 7.94, 7.91, 7.98, 7.94 (RP-HPLC-\( k' \) correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 7.07 (generator column-GC, Larsen et al. 1992)
- 7.51 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:
- 13.09, 11.79 (0, 20°C, multi-column GC-\( k' \) correlation, Zhang et al. 1999)
- 11.81 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \):
- 5.71; 7.24 (zebrafish: \( \log BCF_w \) wet wt basis; \( \log BCF_l \) lipid wt basis, Fox et al. 1994)
- 2.60–4.85 (various marine species, mean dry weight BCF, Hope et al. 1998)
- 4.37–5.67 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, \( \log K_{OC} \):
- 7.72 (suspended particulate matter, calculated-\( K_{OW} \), Burkhard 1984)
- 6.15, 5.92, 5.83, 5.69 (marine humic substances, in concentrations of 5, 10, 20, 40 mg L\(^{-1} \) DOC, reported as association coefficient \( \log K_a \), Lara & Ernst 1989)
- 6.152; 6.133 (marine humic substances of 5 mg L\(^{-1} \) DOC, quoted; calculated-MCI \( \chi \), reported as \( \log K_a \), Sabljic et al. 1989)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

<table>
<thead>
<tr>
<th>Fate Type</th>
<th>Rate Constant</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volatilization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Photolysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrolysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxidation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Biodegradation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Biotransformation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
- \( k_2 > 0.0007 \text{ d}^{-1} \) (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
- \( k_1 = 4940 \text{ d}^{-1} \); \( k_2 = 0.00958 \text{ d}^{-1} \) (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- \( k_2 = 0.016 \text{ d}^{-1} \) with \( t_{1/2} = 45 \text{ d} \) and \( k_2 = 0.013 \text{ d}^{-1} \) with \( t_{1/2} = 53 \text{ d} \) for food concn of 20 ng/g and 141 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- \( k_2 = 0.005 \text{ d}^{-1} \) with \( t_{1/2} = 140 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k_2 = 0.005 \text{ d}^{-1} \) with \( t_{1/2} = 148 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:

Biota: \( t_{1/2} > 1000 \text{ d} \) in rainbow trout, and \( t_{1/2} = 84 \text{ d} \) in its muscle (Niimi & Oliver 1983)

Depuration \( t_{1/2} = 45–53 \text{ d} \) in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

Depuration \( t_{1/2} = 140 \text{ d} \) for high-dose treatment, \( t_{1/2} = 148 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
**Polychlorinated Biphenyls (PCBs)**

**7.1.1.207 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl (PCB-207)**

![Chemical Structure](image)

**Common Name:** 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl  
**Synonym:** PCB-207, 2,2′,3,3′,4,4′,5,6,6′-nonochloro-1,1′-biphenyl  
**Chemical Name:** 2,2′,3,3′,4,4′,5,6,6′-nonachlorobiphenyl

**CAS Registry No:** 52663-79-3  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{Cl}\textsubscript{9}  
**Molecular Weight:** 464.213

**Melting Point** (°C):
- 161 (calculated, Abramowitz & Yalkowsky 1990)

**Boiling Point** (°C):

**Density (g/cm\(^3\)):**
- 372.7 (calculated-Le Bas method at normal boiling point)

**Molar Volume (cm\(^3\)/mol):**
- 4.64 × 10\(^{-3}\), 3.29 × 10\(^{-3}\), 4.04 × 10\(^{-5}\), 3.77 × 10\(^{-5}\) (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 3.17 × 10\(^{-5}\), 4.99 × 10\(^{-5}\) (supercooled liquid P\(_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

**Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):**

**Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):**

**Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:**

**Water Solubility (g/m\(^3\) or mg/L at 25°C):**
- 0.00167 (supercooled liquid S\(_L\), calculated-TSA, Burkhard et al. 1985b)
- 4.64 × 10\(^{-3}\), 3.29 × 10\(^{-3}\), 4.04 × 10\(^{-5}\), 3.77 × 10\(^{-5}\) (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 0.000058 (calculated-TSA, Abramowitz & Yalkowsky 1990)
- 2.10 × 10\(^{-3}\) (calculated-MCI \(\chi\), Patil 1991)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**
- 1.47 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RI correlation, Burkhard et al. 1985a)
- 1.30 × 10\(^{-4}\) (supercooled liquid P\(_L\), GC-RI correlation, Burkhard et al. 1985b)
- 3.17 × 10\(^{-5}\), 4.99 × 10\(^{-5}\) (supercooled liquid P\(_L\), GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

**Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):**
- 35.97 (calculated-P/C, Burkhard et al. 1985b)
- 17.13 (calculated-QSPR, Dunnivant et al. 1992)
- 0.717 (calculated-QSPR, Achman et al. 1993)
- 97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

\[
\ln K_{AW} = -\Delta H_{\text{fus}}/R + \Delta S_{\text{fus}}/R; \quad R \text{ is the ideal gas constant, } \Delta H_{\text{fus}} = 145 \pm 7 \text{ kJ/mol, } \Delta S_{\text{fus}} = 0.46 \pm 0.04 \text{ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004}
\]

**Octanol/Water Partition Coefficient, log \(K_{ow}\):**
- 7.94 (calculated-TSA, Burkhard 1984)
- 7.84, 7.97, 7.85, 7.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 7.52 (generator column-GC, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 7.74 (calculated-TSA, Hawker & Connell 1988a)
- 7.80 (calculated-MCI \(\chi\), Patil 1991)
- 7.88 (recommended, Sangster 1993)
- 7.6190 (calculated-molecular properties MNDO-AM1, Makino 1998)
- 7.77 (calculated-QSPR, Yeh & Hong 2002)
Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated:

- 12.60, 11.26 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 11.94 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, \( \log BCF \):

- 2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.02–6.29 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, \( \log K_{OC} \):

- 7.74 (suspended particulate matter, calculated-\( K_{OW} \), Burkhard 1984)
- 5.98, 5.77, 5.67, 5.44 (marine humic substances, in concentrations of 5, 10, 20, 40 mg L\(^{-1}\) DOC, reported as association coefficient \( K_a \), Lara & Ernst 1989)
- 5.98, 5.97 (marine humic substances of 5 mg L\(^{-1}\) DOC, quoted; calculated-MCI \( \chi \), reported as \( K_h \), Sabljic et al. 1989)
- 6.39, 6.17, 6.19 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

- \( k_1 = 0.004 \text{ d}^{-1} \) with \( t_{1/2} = 162 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- \( k_1 = 0.004 \text{ d}^{-1} \) with \( t_{1/2} = 155 \text{ d} \) (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
  - Biota: depuration \( t_{1/2} = 162 \text{ d} \) for high-dose treatment, \( t_{1/2} = 155 \text{ d} \) for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
7.1.1.208 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl (PCB-208)

Common Name: 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl
Synonym: PCB-208, 2,2′,3,3′,4,5,5′,6,6′-nonachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6,6′-nonachlorobiphenyl
CAS Registry No: 52663-77-1
Molecular Formula: C_{12}H_{Cl9}
Molecular Weight: 464.213
Melting Point (°C): 180.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
372.7 (calculated-Le Bas method at normal boiling point)
276.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 22.60 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K): 49.45 (Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0298 (mp at 180.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.80 × 10⁻⁵ (generator column-GC/ECD, Miller et al. 1984,1985)
6.87 × 10⁻⁵, 4.64 × 10⁻⁵, 6.87 × 10⁻⁵, 3.95 × 10⁻⁵, 4.97 × 10⁻⁵ (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.74 × 10⁻⁷ (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.78 × 10⁻⁶ (GC-RI correlation, Burkhard et al. 1985a)
1.22 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.08 × 10⁻⁴, 6.62 × 10⁻⁵ (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.19 × 10⁻⁵ (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 5127/(T/K) + 12.68 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
32.53 (calculated-P/C, Burkhard et al. 1985b)
9.75 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
ln K_{AW} = −ΔH_{f}/RT + ΔS_{f}/R; R is the ideal gas constant, ΔH_{f} = 145 ± 7 kJ/mol, ΔS_{f} = 0.46 ± 0.04 kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, log K_{ow}:
7.92 (calculated-TSA, Burkhard 1984)
8.16 (generator column-GC/ECD, Miller et al. 1984,1985)
9.05 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
7.72, 7.87, 7.69, 7.78 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
8.18 (calculated-TSA, Hawker & Connell 1988a)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 12.57, 11.26 (0, 20°C, multi-column GC-$k'$ correlation, Zhang et al. 1999)
- 11.71 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 7.72 (suspended particulate matter, calculated-$K_{OW}$, Burkhard 1984)
- 5.974 (marine humic substances 5 mg/L of DOC, reported as association coefficient log $K_a$, calculated-molecular connectivity indices $\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 0.005 \text{ d}^{-1}$ with $t_\text{½} = 139 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
  - $k_1 = 0.005 \text{ d}^{-1}$ with $t_\text{½} = 152 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: depuration $t_\text{½} = 139 \text{ d}$ for high-dose treatment, $t_\text{½} = 152 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
Polychlorinated Biphenyls (PCBs)

7.1.1.209 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl (PCB-209)

![Chemical Structure of PCB-209]

Common Name: 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl
Synonym: PCB-209
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6,6′-decachlorobiphenyl
CAS Registry No: 2051-24-3
Molecular Formula: C_{12}Cl_{10}
Molecular Weight: 498.658
Melting Point (°C):
309 (Lide 2003)
Boiling Point (°C):

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>1.507</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>393.6</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔH_{fus} (kJ/mol)</td>
<td>28.79, 39.434, 38.16</td>
</tr>
<tr>
<td>Entropy of Fusion, ΔS_{fus} (J/mol K)</td>
<td>49.37, 49.37, 3478</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C)</td>
<td>0.015, 1.6 × 10^{-5}</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C)</td>
<td>1.4 × 10^{-5}, 4.0 × 10^{-5}</td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC
Henry’s Law Constant (Pa m³/mol at 25°C):

- 100 (estimated, Mackay et al. 1983)
- 12.46 (calculated-P/C, Burkhard et al. 1985b)
- 20.84 (calculated-P/C, Shiu & Mackay 1986; Shiu et al. 1987)
- 40.0 (calculated-QSPR, Dunnivant et al. 1992)
- 97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

\[ \ln K_{AW} = -\Delta H_d/R + \Delta S_d/R; \]  
\[ R \text{ is the ideal gas constant, } \Delta H_d = 145 \pm 7 \text{ kJ/mol, } \Delta S_d = 0.46 \pm 0.04 \text{ kJ/mol-K} \] (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 11.19 (Hansch & Leo 1979)
- 9.60 (TLC-RT correlation, Bruggeman et al. 1982; 1984)
- 8.26 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 8.20 (generator column-HPLC, Woodburn et al. 1984)
- 8.20 (shake flask/slow stirring-GC, Brooke et al. 1986)
- 8.20 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
- 8.28, 8.37, 8.41, 8.28 (RP-HPLC-k’ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 9.45, 11.2 (calculated-UNIFAC activity coeff., \( \pi \) const. or f const., Banerjee & Howard 1988)
- 8.274 ± 0.001 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- > 9.0 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
- 8.24 (HPLC-retention indices correlation, Noegrohati & Hammers 1992)
- 8.27 (recommended, Hansch et al. 1995)
- 7.95 ± 0.68 (flask/slow stirring-SPME/GC, Paschke et al. 1998)
- 7.59 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated:

- 13.36, 1.96 (0, 20°C, multi-column GC-k’ correlation, Zhang et al. 1999)
- 12.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log \( BCF \) at 25°C or as indicated:

- 5.48 (guppy, 3.5% extractable lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
- 7.0 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
- 1.48, 1.41 (human fat of lipid basis, calculated-\( K_{OW} \), Geyer et al. 1987)
- 1.38, 1.32 (human fat of wet wt. basis, calculated-\( K_{OW} \), Geyer et al. 1987)
- 4.02 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
- 4.02 (guppy, calculated-\( C_p/W \) or \( k_1/k_2 \), Connell & Hawker 1988; Hawker 1990)

© 2006 by Taylor & Francis Group, LLC
Polychlorinated Biphenyls (PCBs) 1997

5.07 (guppy, estimated, Banerjee & Baughman 1991)
5.44; 6.97 (22°C, zebrafish: log BCF<sub>w</sub> wet wt basis; log BCF<sub>L</sub> lipid wt basis, Fox et al. 1994)
2.65–4.54 (various marine species, mean dry wt. BCF; Hope et al. 1998)
> 5.44, > 6.97 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.53, > 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.95, 8.26 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 3.97 (human, steady-state not reached during whole life: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:
13 (trout in Lake Ontario, Niimi 1996)
0.047, 0.42, 0.10 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K<sub>OC</sub>:
8.09 (suspended particulate matter, calculated-K<sub>OW</sub>, Burkhard 1984)
6.19, 5.99, 5.83, 5.61 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K<sub>OC</sub>, Lara & Ernst 1989)
6.19, 6.17 (marine humic substances of 5 mg L<sup>–1</sup> DOC, quoted; calculated-MCI χ<sub>OC</sub>, reported as log K<sub>OC</sub>, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:
Volatilization/Evaporation: 8.5 × 10<sup>–7</sup> g m<sup>–1</sup> h<sup>–1</sup> (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:
k<sub>2</sub> > 0.0007 d<sup>–1</sup> (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k<sub>1</sub> = 40 d<sup>–1</sup>; k<sub>2</sub> = 0.004 d<sup>–1</sup> (guppy, Bruggeman et al. 1984)
k<sub>1</sub> = 600 d<sup>–1</sup> (guppy, Opperhuizen 1986)
log k<sub>1</sub> = 1.60 d<sup>–1</sup>; log 1/k<sub>2</sub> = 2.39 d (fish, quoted, Connell & Hawker 1988)
k<sub>1</sub> = 3640 d<sup>–1</sup>; k<sub>2</sub> = 0.0132 d<sup>–1</sup> (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k<sub>2</sub> = 0.013 d<sup>–1</sup> with t<sub>1/2</sub> = 52 d and k<sub>2</sub> = 0.013 d<sup>–1</sup> with t<sub>1/2</sub> = 52 d for food concn of 62 ng/g and 688 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k<sub>C</sub> = 0.005 d<sup>–1</sup> with t<sub>1/2</sub> = 127 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k<sub>1</sub> = 0.005 d<sup>–1</sup> with t<sub>1/2</sub> = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYP<sub>IA</sub>-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: t<sub>1/2</sub> > 1000 d in rainbow trout, and t<sub>1/2</sub> = 122 d its muscle (Niimi & Oliver 1983);
t<sub>1/2</sub> = 175 d in guppy (Bruggeman et al. 1984).
Depuration t<sub>1/2</sub> = 52 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration t<sub>1/2</sub> = 127 d for high-dose treatment, t<sub>1/2</sub> = 149 d for high-dose + enzyme CYP<sub>IA</sub>-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
TABLE 7.1.1.209.1  
Reported aqueous solubilities and vapor pressures of decachlorobiphenyl at various temperatures and the reported empirical temperature dependence equations

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dickhut et al. 1986</td>
<td>Burkhard et al. 1984</td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>25</td>
<td>6.48 × 10⁻⁷</td>
</tr>
<tr>
<td>60</td>
<td>8.38 × 10⁻⁶</td>
</tr>
<tr>
<td>70</td>
<td>1.63 × 10⁻⁵</td>
</tr>
<tr>
<td>80</td>
<td>4.95 × 10⁻⁵</td>
</tr>
<tr>
<td>ln x = A – B/(T/K)</td>
<td>log (P/Pa) = A – B/(T/K)</td>
</tr>
<tr>
<td>A</td>
<td>-4.608</td>
</tr>
<tr>
<td>B</td>
<td>8010.6</td>
</tr>
</tbody>
</table>

enthalpy of solution:

ΔH_{sol}/(kJ mol⁻¹) = 66.6 ± 4.9 for 40–80°C

ΔH_{subl}/(kJ mol⁻¹) = 101.7

FIGURE 7.1.1.209.1  
Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2’,3,3’,4,4’,5,5’,6,6’-decachlorobiphenyl (PCB-209).
7.1.2 Isomer Groups

7.1.2.1 Monochlorobiphenyl

Common Name: Monochlorobiphenyl
Synonym: Dowtherm G
Chemical Name: monochlorobiphenyl
CAS Registry No: 27323-18-8
Molecular Formula: C_{12}H_9Cl
No. of Isomers: 3
Molecular Weight: 188.652
Melting Point (°C):
  25–77.9 (Shiu et al. 1987)
Boiling Point (°C): 285
Chlorine Content: 18.79% (Hutzinger et al. 1974)
Density (g/cm³): 1.1
Molar Volume (cm³/mol):
  205.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
  0.30–1.0 (Mackay et al. 1983)
  0.301–1.0 (Shiu et al. 1987)
Water Solubility (g/m³ or mg/L at 25°C):
  0.06–1.5 (selected, Mackay et al. 1983)
  7.20 (selected, supercooled liq., Mackay et al. 1983a)
  0.795–6.17, 4.08 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard et al. 1986)
  1.2–5.5 (selected, Shiu et al. 1987)
  2.5–6.73 (selected, supercooled liquid, Shiu et al. 1987)
  1.2–9.5 (selected, Formica et al. 1988)
  4.0 (selected, Metcalfe et al. 1988)
  1.2–5.5 (quoted range of individual congeners, Luthy et al. 1997)
Vapor Pressure (Pa at 25°C):
  1.1–5.6 (selected, Mackay et al. 1983a)
  2.30 (supercooled liquid P_{liq}, Mackay et al. 1983a)
  1.32 (selected, supercooled liq., Bopp 1983)
  1.10 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
  0.271–2.04 (selected, solid, Shiu et al. 1987)
  0.9–2.5 (selected, supercooled liquid, Shiu et al. 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
  79.3 (calculated-P/C, Bopp 1983)
  58–74 (calculated, Mackay et al. 1983a)
  60.0 (selected, Mackay et al. 1983a,b)
  42.56–75.55 (calculated, Shiu et al. 1987)
Octanol/Water Partition Coefficient, log K_{ow}:
  4.66 (selected, Mackay et al. 1983b)
  4.70 (selected, Mackay 1986; Metcalfe et al. 1988)
  4.3–4.6 (selected, Shiu et al. 1987)
  4.73 (calculated-no. Cl atoms, Formica et al. 1988)
  4.50 (quoted, Luthy et al. 1997)
Bioconcentration Factor, log BCF:
3.40 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log $K_{OC}$:

Half-Lives in the Environment:
- Air: atmospheric photodegradation, 0.62–1.4 d (Dilling et al. 1983); calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for monochlorobiphenyls (Kwok et al. 1995).
- Surface water: 1.4–4.9 d in Lake Michigan (Neely 1983); 2–3 d for river water (Bailey et al. 1983).
- Groundwater:
- Sediment:
- Soil:
- Biota:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- Volatilization/Evaporation: $k = 0.25$ g/m² h (Mackay 1986; Metcalfe et al. 1988).
- Photolysis: $t_{1/2} = 0.62–1.4$ d for photodegradation in the atmosphere (Dilling et al. 1983).
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference:
  - $k_{OH}$(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}$(calc) = $(3.1 – 4.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp., and the tropospheric lifetime was calculated to be 5–11 d for monochlorobiphenyls (Atkinson 1987)
  - $k_{OH}$(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, and $k_{OH}$(calc) = $(3.2 – 4.6) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. for reaction with monochlorobiphenyls, the tropospheric lifetime was calculated to be 2.7–5.1 d (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, $7 \times 10^{-8}$ nmol cell⁻¹ h⁻¹ (Furukawa et al. 1978; selected, NAS 1979); time for 50% biodegradation of an initial concentration of 1–100 µg/L by river dieaway test is about 2–5 d (Bailey et al. 1983).

Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
7.1.2.2 Dichlorobiphenyl

Common Name: Dichlorobiphenyl
Synonym:
Chemical Name: dichlorobiphenyl
CAS Registry No: 25512-42-9
Molecular Formula: C\textsubscript{12}H\textsubscript{8}Cl\textsubscript{2}
No. of Isomers: 12
Molecular Weight: 223.098

Melting Point (°C):
- 24.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; quoted, Metcalfe et al. 1988)

Boiling Point (°C):
- 312 (Shiu & Mackay 1986)

Chlorine Content: 31.77%

Density (g/cm\textsuperscript{3} at 20°C): 1.30

Molar Volume (cm\textsuperscript{3}/mol):
- 226.4 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
- 0.06–1.5 (Mackay et al. 1983)
- 0.059–1.0 (Shiu et al. 1987)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 0.22 (quoted, Bopp 1983)
- 0.06–1.5, 2.20 (solid, supercooled liquid, Mackay et al. 1983a)
- 0.898–1.96, 1.60 (exptl. range, calculated-UNIFAC, converted from log $\gamma$, Burkhard & Kuehl 1986)
- 1.6 (Mackay 1986; quoted, Metcalfe et al. 1988)
- 0.06–2.0, 1.02–2.26 (selected, solid, supercooled liquid, Shiu et al. 1987)
- 0.06–2.0 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
- 0.223 (quoted, supercooled liquid, Bopp 1983)
- 0.60 (quoted, supercooled liquid, Mackay et al. 1983a)
- 0.03–0.36 (Mackay et al. 1983)
- 0.24 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
- 0.0018–0.279, 0.008–0.60 (solid, supercooled liquid, Shiu et al. 1987)

Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):
- 153.6 (calculated-P/C, Bopp 1983)
- 60.0 (Mackay et al. 1983a,b)
- 97.0 (calculated-P/C, Mackay et al. 1983a)
- 17–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
- 5.19 (Mackay et al. 1983a,b)
- 5.10 (Mackay 1986; Metcalfe et al. 1988)
- 4.9–5.3 (selected, Shiu et al. 1987)
- 5.13 (calculated-chlorine atoms, Formica et al. 1988)
- 5.10 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
- 3.89 (biota, Mackay et al. 1983b)
- 3.80 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
- 4.10 (calculated-MCI $\chi$, Koch 1983)
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 0.065$ g m$^{-2}$ h$^{-1}$ (selected, Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated,*data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.4 - 2.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 8–17 d at room temp. (Atkinson 1987)

$k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, the tropospheric lifetime is calculated to be 3.4–7.2 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, $6 \times 10^{-8}$ nmol cell$^{-1}$·h$^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979);

$t_{1/2} \approx 2–3$ d for degradation, using river water dieaway test (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the calculated rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 2–3$ d (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:
Polychlorinated Biphenyls (PCBs)

7.1.2.3 Trichlorobiphenyl

Common Name: Trichlorobiphenyl
Synonym:
Chemical Name: trichlorobiphenyl
CAS Registry No: 25323-68-6
Molecular Formula: \( C_{12}H_{7}Cl_{3} \)
No. of Isomers: 24
Molecular Weight: 257.543
Melting Point (°C):
28–87  (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
337  (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 41.4%
Density (g/cm³):
Molar Volume (cm³/mol):
247.3  (calculated-Le Bas method at normal boiling point Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), \( F \):
0.24–0.65  (Mackay et al. 1983)
0.244–0.651 (Shiu et al. 1987)
Water Solubility (g/m³ or mg/L at 25°C):
0.05  (Neely 1980)
0.15–0.64, 0.67(solid, supercooled liquid, Mackay et al. 1983)
0.0654–1.09 (exptl. range, calculated-UNIFAC, converted from log \( \gamma \), Burkhard & Kuehl 1986)
0.65  (quoted, Mackay 1986; Metcalfe et al. 1988)
0.015–0.40  (selected, Shiu et al. 1987)
0.015–0.40  (quoted, Formica et al. 1988)
0.015–0.40  (quoted range for individual congeners, Luthy et al. 1997)
Vapor Pressure (Pa at 25°C):
0.200  (Neely 1980)
0.0375  (supercooled liquid, Bopp 1983)
0.01–0.27, 0.20(solid, supercooled liquid, quoted, Mackay et al. 1983)
0.054  (average, liquid, Mackay 1986; Metcalfe et al. 1988)
0.0136–0.143, 0.003–0.022 (solid, supercooled liquid, Shiu et al. 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
81.76  (calculated-P/C, Bopp 1983)
82–102  (calculated-P/C, Mackay et al. 1983)
77  (selected, Mackay et al. 1983)
24.3–92.2  (calculated-P/C, Shiu et al. 1987)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
5.76  (Mackay et al. 1983)
5.50  (Mackay 1986; Metcalfe et al. 1988)
5.5–5.9  (selected, Shiu et al. 1987)
5.53  (calculated-chlorine atoms, Formica et al. 1988)
5.80  (quoted mean value of isomers, Luthy et al. 1997)
Bioconcentration Factor, log BCF:
4.20  (fish, Mackay 1986; Metcalfe et al. 1988)
4.70  (calculated-MCI \( \chi \), Koch 1983)
Sorption Partition Coefficient, log $K_{OC}$:

Sorption Partition Coefficient, log $K_P$:

- 3.34 (lake sediment, calculated, Formica et al. 1988)
- 3.50 (calculated-MCI $\chi$, Koch 1983)

Environmental Fate Rate Constants, $k$, or Half Lives, $t_{1/2}$:
- Volatilization/Evaporation: $k = 0.017$ g m$^{-2}$ h$^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = (0.7 – 1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 14–30 d at room temp. (Atkinson 1987)
  - $k_{OH}(calc) = (1.0 – 2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radicals for trichlorobiphenyls, the tropospheric lifetime is calculated to be 6.9–15 d (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, $5 \times 10^{-8}$ nmol cell$^{-1}$·h$^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
- tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: estimated $t_{1/2} = 134$ h from fish in simulated ecosystem (Neely 1980).
7.1.2.4 Tetrachlorobiphenyl

Common Name: Tetrachlorobiphenyl
Synonym:
Chemical Name: tetrachlorobiphenyl
CAS Registry No: 26914-33-0
Molecular Formula: C₁₂H₆Cl₄
No. of Isomers: 42
Molecular Weight: 291.988
Melting Point (°C): 47–180 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C): 360 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 48.6%
Density (g/cm³ at 20°C): 1.5
Molar Volume (cm³/mol): 268.2 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, $\Delta H_{\text{ fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{ fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{ fus}} = 56$ J/mol K), F:
0.1–0.68 (Mackay et al. 1983)
0.029–0.606 (Shiu et al. 1987)
Water Solubility (g/m³ or mg/L at 25°C):
0.05 (Neely 1980)
0.0008–0.17 (Mackay et al. 1983)
0.017 (McCall et al. 1983)
0.02–0.0955, 0.224 (exptl. range, calculated-UNIFAC, converted from log $\gamma$, Burkhard & Kuehl 1986)
0.26 (quoted, Mackay 1986; Metcalfe et al. 1988)
0.0043–0.10 (selected, Shiu et al. 1987)
0.039–0.38 (selected, supercooled liquid, Shiu et al. 1987)
0.001–0.10 (Formica et al. 1988)
0.001–0.10 (quoted range for individual congeners, Luthy et al. 1997)
Vapor Pressure (Pa at 25°C):
0.0653 (Neely 1980)
0.0064 (supercooled liquid, Bopp 1983)
0.003–0.104 (Mackay et al. 1983)
0.06 (supercooled liquid, Mackay et al. 1983)
0.0653 (McCall et al. 1983)
0.012 (Mackay 1986; Metcalfe et al. 1988)
5.9 × 10⁻⁵ – 5.4 × 10⁻³ (selected, Shiu et al. 1987)
0.002 (selected, supercooled liquid, Shiu et al. 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
34.69 (calculated-P/C, Bopp 1983)
75–94 (calculated-P/C, Mackay et al. 1983)
76.0 (Mackay et al. 1983)
1.72–47.59 (calculated-P/C, Shiu et al. 1987)
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
6.35 (suggested, Mackay et al. 1983)
5.90 (Mackay 1986, Metcalfe et al. 1988)
5.6–6.5 (selected, Shiu et al. 1987)
Bioconcentration Factor, log BCF:
- 3.98 (pinfish, Branson et al. 1975; quoted, Waid 1986)
- 3.95 (trout, Branson et al. 1975; quoted, NAS 1979)
- 4.79 (McCall et al. 1983)
- 4.60 (fish, Mackay 1986; Metcalfe et al. 1988)
- 5.30 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K\textsubscript{OC}:
- 4.51 (correlated, McCall et al. 1983)
- 3.43–5.11 (correlated of literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, t\textsubscript{1/2}:
Volatilization/Evaporation: \( k = 4.2 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1} \) (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\textsubscript{3}, radical and \( k_{\text{O}_3} \) with O\textsubscript{3} or as indicated, *data at other temperatures see reference:
\( k_{\text{OH}}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated tropospheric lifetime of 25–60 d at room temp. (Atkinson 1987)
\( k_{\text{OH}}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \) for reaction with OH radicals for tetrachlorobiphenyls, the tropospheric lifetime is calculated to be 8.5–40 d (Kwok et al. 1995).
Hydrolysis:
Biodegradation: rate of degradation for both rings substituted with chlorine using species of Alcaligenes and Acinetobacter, \( 2.5 \times 10^{-8} \text{ nmol cell}^{-1} \text{ h}^{-1} \) (Furukawa et al. 1978; selected, NAS 1979); no degradation by river dieaway test after 98 d of incubation (Bailey et al. 1983).
Biotransformation:
Bioconcentration, Uptake (k\textsubscript{1}) and Elimination (k\textsubscript{2}) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil: volatilization t\textsubscript{1/2} ~ 10 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).
Biota: estimated t\textsubscript{1/2} = 139 h from fish in simulated ecosystem (Neely 1980).
7.1.2.5 Pentachlorobiphenyl

Common Name: Pentachlorobiphenyl
Synonym:
Chemical Name: pentachlorobiphenyl
CAS Registry No: 25429-29-2
Molecular Formula: C_{12}H_{5}Cl_{5}
No. of Isomers: 46
Molecular Weight: 326.433

Melting Point (°C):
- 23.5–124 (Shiu et al. 1987)
- 76.5–124 (Shiu & Mackay 1986; Metcalfe et al. 1988)

Boiling Point (°C):
- 381 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 54.4%

Density (g/cm³ at 20°C): 1.50

Molar Volume (cm³/mol):
- 289.1 (Le Bas method at normal boiling point, Shiu & Mackay 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
- 0.1–0.31 (Mackay et al. 1983)
- 0.105–0.311 (Shiu et al. 1987)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.01 (Neely 1980)
- 0.004–0.03 (Mackay et al. 1983)
- 0.072 (supercooled liquid, Mackay et al. 1983)
- 0.0338–0.0525, 0.0829 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
- 0.099 (Mackay 1986; Metcalfe et al. 1988)
- 0.004–0.02 (selected, Shiu et al. 1987)
- 0.03–0.11 (selected, supercooled liquid, Shiu et al. 1987)
- 0.004–0.02 (Formica et al. 1988)
- 0.024 (selected average value of isomers, Mackay 1989)
- 0.004–0.02 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
- 0.01026 (Neely 1980)
- 0.00111 (supercooled liquid, Bopp 1983)
- 0.015 (supercooled liquid, Mackay et al. 1983)
- 0.004–0.03 (Mackay et al. 1983)
- 0.0026 (Mackay 1986; Metcalfe et al. 1988)
- 0.000304–0.0093 (selected, Shiu et al. 1987)
- 0.0023–0.051 (selected, supercooled liquid, Shiu et al. 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 68.0 (suggested, Mackay et al. 1983)
- 17.34 (calculated-P/C, Bopp 1983)
- 24.8–151.4 (selected, Shiu et al. 1987)
- 12.2 (calculated, Mackay 1989)

Octanol/Water Partition Coefficient, log K_{ow}:
- 6.85 (suggested, Mackay et al. 1983)
- 6.33 (calculated-chlorine atoms, Formica et al. 1988)
6.30 (Mackay 1986; Metcalfe et al. 1988)
6.2–6.5 (selected, Shiu et al. 1987)
6.60 (selected, Mackay 1989)
6.40 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
5.0 (fish, Mackay 1986; Metcalfe et al. 1988)
5.30 (Mackay 1989)
5.90 (calculated-MCI $\chi$, Koch 1983)

Sorption Partition Coefficient, log $K_{OC}$:
6.21 (calculated, 0.41$K_{OW}$, Mackay 1989)

Sorption Partition Coefficient, log $K_p$:
4.15 (lake sediment, calculated-$K_{OW}$ $f_{OC}$, Formica et al. 1988)
4.51 (calculated-MCI $\chi$, Koch 1983)

Environmental Fate Rate Constants, $k$, and Half Lives, $t_{1/2}$:
Vaportalization /Evaporation: $k = 1.0 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2 – 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., with a calculated tropospheric lifetime of 60–120 d (Atkinson 1987);

$k_{OH}(\text{calc}) = (0.3 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radicals for pentachlorobiphenyls, the tropospheric lifetime is calculated to be 16–48 d (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2} = 0.62–1.4 \text{ d}$ for atmospheric photodegradation (Dilling et al. 1983);
calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radicals for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radicals for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil: volatilization $t_{1/2} = 25 \text{ d}$ from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).
Biota: estimated $t_{1/2} = 226 \text{ d}$ from fish in simulated ecosystem (Neely 1980).
7.1.2.6 Hexachlorobiphenyl

Common Name: Hexachlorobiphenyl

Chemical Name: hexachlorobiphenyl

CAS Registry No: 26601-64-9

Molecular Formula: C₁₂H₄Cl₆

No. of Isomers: 42

Molecular Weight: 360.878

Melting Point (°C):
- 85–160 (Shiu et al. 1987)
- 77–150 (Shiu & Mackay 1986; Metcalfe et al. 1988)

Boiling Point (°C):
- 400 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 62.77% (Hutzinger et al. 1974)

Density (g/cm³ at 20°C): 1.60

Molar Volume (cm³/mol):
- 310.0 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔHₘₚ (kJ/mol): 0.06–0.25 (Mackay et al. 1983)

Entropy of Fusion, ΔSₘₚ (J/mol K):
- 0.0582–0.256 (Shiu & Mackay 1986)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0004–0.01, 0.021 (solid, supercooled liquid, Mackay et al. 1983)
- 0.00303–0.0504, 0.00297 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
- 0.038 (Mackay 1986; Metcalfe et al. 1988)
- 0.0004–0.001, 0.0022–0.01 (solid, supercooled liquid, Shiu et al. 1987)
- 0.0004–0.005 (Formica et al. 1988)
- 0.0035 (Mackay & Paterson 1991)
- 0.0004–0.001 (quoted range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
- 0.000182 (supercooled liquid, Bopp 1983)
- 0.0016, 0.005 (solid, supercooled liquid, Mackay et al. 1983)
- 5.8 × 10⁻⁴ (Mackay 1986; Metcalfe et al. 1988)
- 2.0 × 10⁻³ – 1.59 × 10⁻³, 7.0 × 10⁻⁴ – 0.012 (solid, supercooled liquid, Shiu et al. 1987)
- 0.0005 (selected, Mackay & Paterson 1991)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 86.0 (Mackay et al. 1983)
- 6.70 (calculated-P/C, Bopp 1983)
- 11.9–81.8 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log KOW:
- 6.70–7.30 (selected, Shiu et al. 1987)
- 6.70 (selected, Mackay 1986; Metcalfe et al. 1988)
- 6.80 (selected, Mackay & Paterson 1991)
- 7.00 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
- 6.50 (calculated-MCI χ, Koch 1983)
- 5.39 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
- 4.57 (green alga, Mailhot 1987)
Sorption Partition Coefficient, log $K_{OC}$:
4.785–6.869 (correlated literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization/Evaporation: $2.5 \times 10^{-4} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalf et al. 1988).
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  $k_{OH} \text{(calc)} = (0.16 – 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation: degradation rate constants estimated to be $1.5 \times 10^{-5} \text{ h}^{-1}$ in water, soil and sediment (Mackay & Patterson 1991).
- Biotransformation:

Half-Lives in the Environment:
- Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil: volatilization $t_{1/2} = 40 \text{ d}$ from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).
- Biota:
7.1.2.7 Heptachlorobiphenyl

Common Name: Heptachlorobiphenyl
Synonym:
Chemical Name: heptachlorobiphenyl
CAS Registry No: 28655-71-2
Molecular Formula: C_{12}H_3Cl_7
No. of Isomers: 24
Molecular Weight: 395.323
Melting Point (°C):
122.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
417 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 62.77% (Hutzinger et al. 1974)
Density (g/cm³ at 20°C): 1.70
Molar Volume (cm³/mol):
330.9 (Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0596–0.109 (Shiu et al. 1987)
Water Solubility (g/m³ or mg/L at 25°C):
0.0005, 0.006 (solid, supercooled liquid, Mackay et al. 1983)
0.00816–0.0205, 0.011 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.014 (Mackay 1986; Metcalfe et al. 1988)
0.00045–0.002, 0.0076–0.018 (solid, supercooled liquid, selected, Shiu et al. 1987)
0.00046–0.002 (Formica et al. 1988)
Vapor Pressure (Pa at 25°C):
0.0015 (supercooled liquid, Mackay et al. 1983)
1.3 × 10⁻⁴ (Mackay 1986; Metcalfe et al. 1988)
2.73 × 10⁻³, 2.5 × 10⁻⁴ (solid, supercooled liquid, Shiu et al. 1987)
Henry’s Law Constant (Pa m³/mol):
100.0 (Mackay et al. 1983)
5.4 (calculated-P/C, Shiu et al. 1987)
Octanol/Water Partition Coefficient, log K_{ow}:
7.1 (Mackay 1986; Metcalfe et al. 1988)
6.7–7.0 (selected, Shiu et al. 1987)
Bioconcentration Factor, log BCF:
7.10 (calculated-MCI χ, Koch 1983)
5.80 (fish, Mackay 1986; Metcalfe et al. 1988)
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization/Evaporation: k = 6.2 × 10⁻⁵ g m⁻² h⁻¹ (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:

Half-Lives in the Environment:
7.1.2.8 Octachlorobiphenyl

Common Name: Octachlorobiphenyl
Synonym:
Chemical Name: octachlorobiphenyl
CAS Registry No: 31472-83-0
Molecular Formula: C₁₂H₂Cl₈
No. of Isomers: 12
Molecular Weight: 429.768

Melting Point (°C):
159–162 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)

Boiling Point (°C):
432 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 65.98% (Hutzinger et al. 1974)

Density (g/cm³ at 20°C): 1.7

Molar Volume (cm³/mol):
351.8 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔHₖₑₚ (kJ/mol):
Entropy of Fusion, ΔSₖₑₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₖₑₚ = 56 J/mol K), F:
0.0443–0.0474 (Shiu et al. 1987)

Water Solubility (g/m³ or mg/L at 25°C):
0.0002–0.007, 0.020 (solid, supercooled liquid, estimated, Mackay et al. 1983)
0.00345–0.006, 0.00378 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.0055 (Mackay 1986; Metcalfe et al. 1988)
0.0002–0.0003, 0.004–0.0068 (solid, supercooled liquid, Shiu et al. 1987)

Vapor Pressure (Pa at 25°C):
2.8 × 10⁻⁵ (Mackay 1986; Metcalfe et al. 1988)
2.66 × 10⁻⁵, 6.0 × 10⁻³ (solid, supercooled liquid, selected, Shiu et al. 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
100.0 (suggested, Mackay et al. 1983)
38.08 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log Kₐₕₖ:
8.55 (Mackay et al. 1983)
7.50 (Mackay 1986; Metcalfe et al. 1988)
7.1 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
6.20 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log Kₐₕₖ:

Environmental Fate Rate Constants, k or Half-Lives, tₕₖ:
Volatilization/Evaporation: k = 1.5 × 10⁻⁵ g m⁻² h⁻¹ (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:
7.1.2.9 Nonachlorobiphenyl

Common Name: Nonachlorobiphenyl
Synonym:
Chemical Name: nonachlorobiphenyl
CAS Registry No: 53742-07-7
Molecular Formula: C₁₂HCl₉
No. of Isomers: 3
Molecular Weight: 464.213
Melting Point (°C):
  182.8–206 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
  445 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 68.73% (Hutzinger et al. 1974)
Density (g/cm³ at 20°C): 1.80
Molar Volume (cm³/mol):
  372.7 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
Entropy of Fusion, ΔSₘₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F:
  0.016 (Mackay et al. 1983)
  0.0163–0.0276 (Shiu et al. 1987)
Solubility (g/m³ or mg/L at 25°C):
  0.0001, 0.0007 (solid, supercooled liquid, Mackay et al. 1983)
  0.000678–0.00148, 0.00145 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
  0.002 (Mackay 1986; Metcalfe et al. 1988)
  0.000018–0.00011, 0.00065–0.0068 (solid, supercooled liquid, selected, Shiu et al. 1987)
Vapor Pressure (Pa at 25°C):
  0.00015 (supercooled liquid, Mackay et al. 1983)
  6.3 × 10⁻⁶ (Mackay 1986; Metcalfe et al. 1988)
Henry’s Law Constant (Pa m³/mol at 25°C):
  100.0 (estimated, Mackay et al. 1983)
Octanol/Water Partition Coefficient, log Kₗₗ:
  9.14 (Mackay et al. 1983)
  7.9 (Mackay 1986; Metcalfe et al. 1988)
  7.2–8.16 (selected, Shiu et al. 1987)
Bioconcentration Factor, log BCF:
  6.60 (fish, Mackay 1986; Metcalfe et al. 1988)
Sorption Partition Coefficient, log Kₗₗ:
Environmental Fate Rate Constants, k or Half-Lives, tₕₜ:
  Volatilization/Evaporation: k = 3.5 × 10⁻⁶ g m⁻² h⁻¹ (Mackay 1986; Metcalfe et al. 1988).
Half-Lives in the Environment:
### 7.1.3 AROCLOR MIXTURES

#### 7.1.3.1 Aroclor 1016

Common Name: Aroclor 1016  
Synonym:  
Chemical Name:  
CAS Registry No: 12674-11-2  
Molecular Formula:  
Average Molecular Weight: 257  
Physical state: mobile oil  
Distillation Range (°C):  
323–356 (NAS 1979; Brinkman & De Kock 1980)  
Chlorine Content: 41%  
Density (g/cm³):  
1.37 (20°C, Brinkman & De Kock 1980)  
1.36–1.37 (25°C, NAS 1979)  
1.33 (Mills et al. 1982)  
1.40 (25°C, Mackay 1986)  
Molar Volume (cm³/mol):  
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
0.22–0.25 (estimated, Tucker et al. 1975)  
0.906 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Lee et al. 1979)  
0.42 (shake flask-GC/ECD, Paris et al. 1978; Callahan et al. 1979; Mackay et al. 1980; Mills et al. 1982)  
0.906 (shake flask-GC/ECD, Lee et al. 1979)  
0.049, 0.490 (shake flask, nephelometric, Hollifield 1979)  
0.085 (Kenaga & Goring 1980)  
0.34 (quoted, Pal et al. 1980)  
0.906 (23°C, shake flask-GC/ECD, Griffin & Chian 1981; quoted, Sklarew & Girvin 1987)  
0.40–0.91 (selected, Mackay et al. 1983)  
0.84 (selected, Mackay 1986; Metcalfe et al. 1988)  
0.332 (quoted, Chou & Griffin 1986)  
Vapor Pressure (Pa at 25°C):  
0.0533 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)  
0.060 (quoted, Mackay et al. 1983)  
0.200 (quoted, supercooled liquid, Mackay et al. 1983)  
0.10 (selected, Mackay 1986; Metcalfe et al. 1988)  
0.12, 0.121 (GC-RT correlation, Foreman & Bidleman 1985)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
1368 (calculated, Paris et al. 1978)  
33.4 (calculated-P/C, Mabey et al. 1982)  
77.0 (calculated, Mackay et al. 1983)  
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:  
$> 5.58$ (shake flask, Chiou et al. 1977; Callahan et al. 1979; Veith et al. 1979a; Kenaga & Goring 1980; Mabey et al. 1982; Mackay 1982)  
4.38 (shake flask-GC, Paris et al. 1978; quoted, Callahan et al. 1979; Ryan et al. 1988)  
5.88 (HPLC-RT correlation, Veith et al. 1979b; Garten & Trabalka 1983)  
3.48 (Pal et al. 1980; Sklarew & Girvin 1987)
4.3–5.48 (quoted, Mills et al. 1982)
4.40–5.80 (selected, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988)
5.31 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:
3.80, 3.81, 3.74 (bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
4.18 (fish in Hudson River, Skea et al. 1979; quoted, Waid 1986)
4.63 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
4.70 (microorganism, calculated-K_{ow}, Mabey et al. 1982)
4.63; 4.56 (fish, quoted; calculated-K_{ow}, Mackay 1982)
0.15 (rodents, Garten & Trabalka 1983)
4.63 (fish, Garten & Trabalka 1983)
4.63 (fathead minnow, quoted, Zaroogian et al. 1985)
4.24, 4.30 (oyster, quoted, Zaroogian et al. 1985)
3.11–4.5 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:
5.26 (calculated-K_{ow}, Mabey et al. 1982)
4.87 (calculated, Sklarew & Girvin 1987)
4.25 (soil, calculated-S, Chou & Griffin 1986)
5.03, 4.97 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{\text{1/2}}$:
Volatilization/Evaporation: volatilization $t_{\text{1/2}} = 9.9$ h (Paris et al. 1978, quoted Callahan et al. 1979);
rate constant $k = 0.031$ g m$^{-2}$ h$^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis: not environmentally significant (Mabey et al. 1982).
Oxidation: calculated rate constant for singlet oxygen, $k << 360$ M$^{-1}$ h$^{-1}$ and $k << 1$ M$^{-1}$ h$^{-1}$ for RO$_2$ (peroxy radical) (Mabey et al. 1982).
Biodegradation: 32.9% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);
33% degraded by activated sludge for 48-h exposure (Tucker et al. 1975; Versar Inc. 1979; quoted, Pal et al. 1980);
rate constant $k = 0.2$ d$^{-1}$ by acclimated activated sludge with $t_{\text{1/2}} = 3.5$ d (Callahan et al. 1979).
96% loss by degradation with Nocardia strain NCIB 10603 and 91% loss with NCIB 10643, both within 52 d; > 98% loss with NCIB 10603 and > 96% loss with NCIB 10643, both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).
Biotransformation: $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12}$ mL cell$^{-1}$ h$^{-1}$, estimated for bacteria transformation in water (Mabey et al. 1982).
Bioconcentration, Uptake (k$^1$) and Elimination (k$^2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $t_{\text{1/2}} = 9.9$ h in 1 m$^3$ water of 1-m deep (Paris et al. 1978; selected, Callahan et al. 1979; Mills et al. 1982)
Groundwater:
Sediment:
Soil: $t_{\text{1/2}} > 50$ d (Ryan et al. 1988).
Sludge: estimated $t_{\text{1/2}} = 15$ d for the volatilization from activated sludge under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).
Biota: $t_{\text{1/2}} \sim 1.2$ yr in fish in Hudson River (Armstrong & Sloan 1985).
7.1.3.2 Aroclor 1221

Common Name: Aroclor 1221
Synonym:
Chemical Name:
CAS Registry No: 11104-28-2
Molecular Formula:
Average Molecular Weight: 192–200.7
Physical State: mobile oil
Distillation Range (°C):
    275–320 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 20.5–21.5%
Density (g/cm³):
    1.182–1.19 (25°C, NAS 1979)
    1.18 (20°C, Brinkman & De Kock 1980)
    1.15 (Callahan et al. 1979; Mills et al. 1982)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    5.00 (Zitko 1970, 1971)
    3.5 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Chou & Griffin 1986)
    15.0 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Pal et al. 1980; Mills et al. 1982)
    3.52 (shake flask-GC/ECD, Lee et al. 1979)
    0.59 (shake flask-nephelometric, Hollifield 1979)
    40.0 (calculated-K_{ow}, Mabey et al. 1982)
    3.50–15.0 (selected, Mackay et al. 1983)

Vapor Pressure (Pa at 25°C):
    0.893 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
    0.93 (Pal et al. 1980)
    0.89 (quoted, Mackay et al. 1983)

Henry’s Law Constant (Pa m³/mol):
    0.750 (Hetling et al. 1978)
    17.23 (calculated-P/C, Mabey et al. 1982)
    60.0 (suggested value, Mackay et al. 1983)
    23.10 (calculated, Burkhard et al. 1985b)

Octanol/Water Partition Coefficient, log K_{ow}:
    2.8 (Monsanto Co. 1972; quoted, Callahan et al. 1979)
    2.81 (Pal et al. 1980)
    4.08 (Callahan et al. 1979; Mabey et al. 1982)
    4.10–4.70 (quoted, Mackay et al. 1980)
    2.78–4.0 (quoted, Mills et al. 1982)
    4.09 (quoted, Chou & Griffin 1986)
    4.09 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:
    3.34 (microorganism, calculated-K_{ow}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
    3.76 (sediment, calculated-K_{ow}, Mabey et al. 1982)
    3.62 (soil, calculated-S, Chou & Griffin 1986)

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

- **Volatileization**: estimated $k \sim 1.74 \text{ mg cm}^{-2} \text{ h}^{-1}$ from liquid substrate at 100°C (Hutzinger et al. 1974; quoted, Pal et al. 1980).

- **Photolysis**: not environmentally significant (Mabey et al. 1982).

- **Hydrolysis**: calculated rate constant for singlet oxygen, $k << 360 \text{ M}^{-1} \text{ h}^{-1}$ and $k << 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO$_2$ (peroxy radical) (Mabey et al. 1982).

- **Oxidation**: 80.6% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980); 81% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980); $k = 0.8 \text{ d}^{-1}$ and $t_{1/2} = 0.9 \text{ d}$ for biodegradation by acclimated activated sludge (Callahan et al. 1979).

- **Biotransformation**: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ rate of transformation for bacteria in water (Mabey et al. 1982).

- **Biodegradation**: 80.6% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980); 81% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980); $k = 0.8 \text{ d}^{-1}$ and $t_{1/2} = 0.9 \text{ d}$ for biodegradation by acclimated activated sludge (Callahan et al. 1979).

- **Biotransformation**: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ rate of transformation for bacteria in water (Mabey et al. 1982).

- **Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants**:

Half-Lives in the Environment:

- **Air**:
  - Surface water:
  - Groundwater:
  - Sediment:
  - Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

- **Sludge**: estimated $t_{1/2} = 12 \text{ d}$ of volatilization from activated sludge to be 12 d under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).

- **Biota**: 

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
7.1.3.3 Aroclor 1232

Common Name: Aroclor 1232
Synonym:

Chemical Name:

CAS Registry No: 11141-16-5

Molecular Formula:

Average Molecular Weight: 221–232.2

Physical State: mobile oil

Distillation Range (°C):

270–325 (NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 32%

Density (g/cm³):

1.260 (20°C, Brinkman & De Kock 1980)
1.27–1.28 (25°C, NAS 1979)
1.24 (Callahan et al. 1979; Mills et al. 1982)

Molar Volume (cm³/mol):

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

1.45 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Chou & Griffin 1986)
1.45 (quoted, Pal et al. 1980; Mackay et al. 1983)
407 (calculated-$K_{\text{OW}}$, Mabey et al. 1982)

Vapor Pressure (Pa at 25°C):

0.54 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
0.533 (quoted, Mills et al. 1982)
0.54 (quoted, Mackay et al. 1983)

Henry’s Law Constant (Pa m³/mol):

60.0 (suggested, Mackay et al. 1980)
1.14 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:

3.2 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
4.54 (Tulp & Hutzinger 1978; Callahan et al. 1979)
3.23 (quoted, Pal et al. 1980)
3.18–4.48 (quoted, Mills et al. 1982)
4.10–5.20 (quoted, Mackay et al. 1983)
4.62 (calculated-S, Chou & Griffin 1986)
4.54 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:

2.54 (microorganism, calculated-$K_{\text{OW}}$, Mabey et al. 1982)

Sorption Partition Coefficient, log $K_{\text{OC}}$:

2.89 (sediment, calculated-$K_{\text{OW}}$, Mabey et al. 1982)
3.85 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).
Oxidation: calculated rate constant for singlet oxygen $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO$_2$ (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{1/2} = 61.4 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 33.4 \text{ d}$ with chitin and $t_{1/2} = 26.8 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: $k \sim 3 \times 10^{-9} \text{ to } 3 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$, estimated rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: aerobic biodegradation $t_{1/2} = 61.4 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 33.4 \text{ d}$ with chitin and $t_{1/2} = 26.8 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:
Sediment:
Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

Biota:
7.1.3.4 Aroclor 1242

Common Name: Aroclor 1242
Synonym:
Chemical Name:
CAS Registry No: 534-692-19
Molecular Formula:
Average Molecular Weight: 261–266.5
Physical State: mobile oil
Distillation Range (°C):
325–366 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 42%
Density (g/cm³):
1.38 (Brinkman & De Kock 1980)
1.30–1.39 (quoted, NAS 1979)
1.35 (Callahan et al. 1979; Mills et al. 1982)
1.40 (quoted, Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm³/mol):

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.20 (Monsanto Co. 1972; quoted, Hutzinger et al. 1974; Tucker et al. 1975; Sawhney 1987)
0.20 (20°C, Nisbet & Sarofim 1972)
0.24 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Brinkman & De Kock 1980; Geyer et al. 1980; Pal et al. 1980; Erickson 1986)
0.045 (shake flask-GC, Lawrence & Tosine 1976)
0.085 (Branson 1977; Kenaga & Goring 1980)
0.703 (23°C, shake flask-GC/ECD, Griffin et al. 1978)
0.34 (shake flask-GC/ECD, Paris et al. 1978)
0.1329 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
0.23 (quoted, Callahan et al. 1979; Mabey et al. 1982)
0.23–0.703 (shake flask-GC, Lee et al. 1979)
0.10 (shake flask-nephelometric, Hollifield 1979)
0.703 (20°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
0.25 (quoted, Eisenreich et al. 1981)
0.34–0.703 (selected, Westcott et al. 1981)
0.10–0.30 (selected, Mills et al. 1982)
0.75 (selected, Mackay 1986; Metcalfe et al. 1988)
0.277 (20°C, calculated from mole fraction, Murphy et al. 1987)
0.097; 0.085–0.34 (21°C, shake flask-GC/ECD; quoted lit. range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0133 (20°C, Nisbet & Sarofim 1972)
0.12 (20°C, extrapolated, Monsanto 1972; NAS 1979)
\[
\log (P_{\text{L}}/\text{mmHg}) = 8.80 - 3500/(T/K) \quad \text{(temp range 150–300°C, from Monsanto 1972, NAS 1979)}
\]
0.055 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983; Bidleman & Christiansen 1979)
0.054 (Callahan et al. 1979; Westcott et al. 1981; Eisenreich et al. 1981; Richardson et al. 1983)
0.054 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
0.040 (38°C, average, Wingender & Williams 1984)
0.076, 0.077 (GC-RT correlation, Foreman & Bidleman 1985)
0.077 (quoted, Mackay et al. 1986)
0.0517 (quoted, Eisenreich 1987)
0.091 (selected, Mackay 1986; Metcalfe et al. 1988)
0.033 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
58.06 (calculated, Mackay & Leinonen 1975)
768 (calculated, Paris et al. 1978)
59.5 (Slinn et al. 1978)
56.74 (calculated-P/C, Eisenreich et al. 1981)
20.27–41.54 (calculated, Westcott et al. 1981)
34.69 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
200.6 (calculated-P/C, Mabey et al. 1982)
22.29 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
40.3 (16°C, calculated-P/C, Richardson et al. 1983)
34.75 (calculated, Burkhard et al. 1985b)
50.0 (calculated, Mackay et al. 1986)
34.45 (calculated-P/C, Eisenreich 1987)
23.0 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)
28.31 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
28.27 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

\[ \log K_{AW} = 12.869 - \frac{4339}{T/K} \] (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
4.11 (Callahan et al. 1979; Mabey et al. 1982; quoted, Ryan et al. 1988)
5.58 (HPLC-RT correlation, Veith et al. 1979a; quoted, Kenaga & Goring 1980)
0.703 (shake flask-GC/ECD, Lee et al. 1979)
3.54 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
4.0–5.6 (quoted, Mills et al. 1982)
4.50–5.80 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
5.90 (Rapaport & Eisenreich 1984)
5.74 (literature mean, Di Toro et al. 1985)
5.29 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, \( \log BCF \):
3.92, 3.65, 3.46(bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
0.08, –0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
3.36 (microorganism, calculated-KOC, Mabey et al. 1982)
0.30, 0.13, –0.11, –0.50, –0.27 (rodent, poultry, sheep, small birds, swine, Garten & Trabalka 1983)
3.20–4.51 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.69, 5.99 (fish 5% lipid in flow-through system: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, \( \log K_{OC} \):
3.80 (sediment, calculated-KOC, Mabey et al. 1982)
4.17 (Lake Michigan sediment, 0.7–3.8% OC, Eadie et al. 1983)
3.36 (calculated, Sklarew & Girvin 1987)
4.09 (soil, calculated-S, Chou & Griffin 1986)
4.30, 4.12, 4.64(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 2.0 to > 10, average, Delle Site 2001)
4.82, 4.74 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
Polychlorinated Biphenyls (PCBs)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$;
- Volatilization/Evaporation: $k = 0.23 \mu g m^{-2} d^{-1}$ with $t_{1/2} = 17 d$ (Baker et al. 1986);
  
  $k = 0.029 g m^{-2} h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

- Photolysis:
  Hydrolysis: not environmentally significant (Mabey et al. 1982).
- Oxidation: calculated rate constant for singlet oxygen, $k << 360 M^{-1} h^{-1}$ and $k << 1 M^{-1} h^{-1}$ for RO$_2$ (peroxy radical) (Mabey et al. 1982).
- Biodegradation: 26.3% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980);
  
  26% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980);
  
  degraded by acclimated activated sludge with a first-order rate constant $k = 0.15 d^{-1}$ and $t_{1/2} = 4.5 d$
  (Callahan et al. 1979).
- 88% loss by degradation with Nocardia strain NCIB 10603, 76% loss with NCIB 10643 both within
  
  52 d; 95% loss with NCIB 10603 and 85% loss with NCIB 10643 both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).

- Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12}$ mL·cell$^{-1}$·h$^{-1}$ for bacteria transformation in water (Mabey et al. 1982).

- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air:
  Surface water: $t_{1/2} = 12 h$ (Paris et al. 1978); volatilization $t_{1/2} \approx 12 h$ at 1 m depth in 1 m$^3$ of water (Mackay &
  
  Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

- Groundwater:

- Sediment:
  Soil: $t_{1/2} > 50 d$ (Ryan et al. 1988).

- Biota:
7.1.3.5  Aroclor 1248

Common Name: Aroclor 1248

Synonym:

Chemical Name:

CAS Registry No: 12672-29-6

Molecular Formula:

Average Molecular Weight: 288–299.5

Physical State: mobile oil

Distillation Range (°C):

340–375 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 48%

Density (g/cm³):

1.44 (20°C, Brinkman & De Kock 1980)
1.40–1.41 (NAS 1979)
1.41 (Callahan et al. 1979)
1.40 (Mackay 1986; Mills et al. 1982; Metcalfe et al. 1988)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ∆Hfus (kJ/mol):

Entropy of Fusion, ∆Sfus (J/mol K):

Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

0.10 (20°C, Nisbet & Sarofim 1972)
0.10 (Monsanto Co. 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
0.043 (26°C, Hutzinger et al. 1974)
0.054 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983, 1986)
0.054 (NAS 1979; Callahan et al. 1979; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Chou & Griffin 1986)
0.060 (shake flask-nephelometry, Hollifield 1979)
0.052 (quoted, Brinkman & De Kock 1980; Erickson 1986)
0.32 (selected, Mackay 1986; Metcalfe et al. 1988)
0.056 (selected, Eisenreich 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.004 (20°C, Nisbet & Sarofim 1972)
0.066 (selected, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; quoted, Mills et al. 1982)
0.11 (20°C, extrapolated, Monsanto 1972; quoted, NAS 1979)
log (P/μmHg) = 8.40 – 3400/(T/K) (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.017 (Branson 1977; Kenaga & Goring 1980)
0.066 (Callahan et al. 1979; Mabey et al. 1982; Mackay et al. 1983)
0.025, 0.024 (GC-RT correlation, Foreman & Bidleman 1985)
0.0085 (selected, Eisenreich 1987)
0.023 (selected, Mackay 1986; Metcalfe et al. 1988)

Henry’s Law Constant (Pa m³/mol):

355.7 (calculated, Mackay & Leinonen 1975)
372 (Slinn et al. 1978)
364 (calculated-P/C, Mabey et al. 1982)
86.0 (calculated-P/C, Mackay et al. 1983)
44.58 (calculated, Burkhard et al. 1985; quoted, Eisenreich 1987)
50.0 (calculated-P/C, Mackay et al. 1986)

Octanol/Water Partition Coefficient, log Kow:

5.75 (Callahan et al. 1979; Kenaga & Goring 1980; Mabey et al. 1982; Chou & Griffin 1986)
Polychlorinated Biphenyls (PCBs)

Bioconcentration Factor, log BCF:
- 4.42 (bluegill sunfish, Stalling & Meyer 1972)
- 4.75-4.79 (channel catfish, Mayer et al. 1977; quoted, Waid 1986)
- 5.08 (fathead minnow, DeFoe et al. 1978; quoted, Waid 1986)
- 4.85 (fathead minnow, 32-d exposure, Veith et al. 1979b)
- 4.86, 4.07 (fish, flowing water, static water, Kenaga & Goring 1980)
- 4.86 (quoted, Bysshe 1982)
- 3.86-4.42, 4.19 (mussel, range, average, Geyer et al. 1982)
- 4.86 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
- 4.85, 4.79 (fish: quoted, calculated-K_{OW}, Mackay 1982)
- 4.85, 0.82, 0.72 (fish, poultry, rodents, Garten & Trabalka 1983)
- 4.5-5.0 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
- 4.80, 6.08 (fathead minnow, male: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.08, 6.08 (fathead minnow, female: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
- 5.44 (sediment, calculated-K_{OW}, Mabey et al. 1982)
- 4.74 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
- Volatilization/Evaporation: k = 8.3 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1} (Mackay 1986; Metcalfe et al. 1988).
- Photolysis: TiO_{2} catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).
- Hydrolysis: not environmentally significant (Mabey et al. 1982).
- Oxidation: calculated rate constant for singlet oxygen, k \ll 360 \text{ M}^{-1} \text{ h}^{-1} and k \ll 1 \text{ M}^{-1} \text{ h}^{-1} for RO_{2} (peroxy radical) (Mabey et al. 1982).
- Biodegradation: aerobic biodegradation t_{1/2} = 77.6 \text{ d} without the addition of polymer chitin, t_{1/2} = 38.6 \text{ d} with chitin and t_{1/2} = 31.9 \text{ d} with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected form the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).
- Biotransformation: estimated k \sim 3 \times 10^{-6} to 3 \times 10^{-12} \text{ mL-cell}^{-1} \text{ h}^{-1} for bacteria transformation in water (Mabey et al. 1982).
- Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
  \log k_2 = -1.92 \text{ d}^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:
- Air:
  Surface water: volatilization t_{1/2} \sim 10 \text{ h} at 1 \text{ m} depth in 1 \text{ m}^3 \text{ water} (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982);
  TiO_{2} catalyzed photolytic process destroyed 80\% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50\% destroyed in sediment suspension within 6 h (Zhang et al. 1993).
- Groundwater:
  Sediment:
  Soil: t_{1/2} > 50 \text{ d} (Ryan et al. 1988).
- Biota:
7.1.3.6 Aroclor 1254

Common Name: Aroclor 1254
Synonym: 
Chemical Name: 
CAS Registry No: 11097-69-1
Molecular Formula: 
Average Molecular Weight: 327–328.4
Physical State: viscous liquid
Distillation Range (°C):
   365–390  (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 54%
Density (g/cm³):
   1.505  (Monsanto 1972)
   1.49–1.50  (65°C, NAS 1979)
   1.54  (20°C Brinkman & De Kock 1980)
   1.50  (Mills et al. 1982; Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm³/mol):
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   0.30  (Zitko 1971)
   0.043  (26°C, Nelson et al. 1972)
   0.050  (20°C, Nisbet & Sarofim 1972)
   0.040  (Monsanto 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
   0.012–0.07  (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Geyer et al. 1980; Mackay et al. 1983, 1986)
   0.056  (shake flask-GC, Haque et al. 1974; quoted, Haque et al. 1980)
   0.0001  (20°C, shake flask-GC/ECD, Schoor 1975)
   0.045  (shake flask-GC, Lawrence & Tosine 1976)
   0.070  (23°C, shake flask-GC/ECD, Griffin et al. 1978)
   0.0242  (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
   0.012  (Brinkman & De Kock 1980; Giam et al. 1980; Pal et al. 1980; Erickson 1986)
   0.010  (Kenaga & Goring 1980)
   0.031  (Callahan et al. 1979; Mabey et al. 1982)
   0.070  (shake flask-GC/ECD, Lee et al. 1979)
   0.057  (shake flask-nephelometry, Hollifield 1979)
   0.070  (23°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
   0.0115  (quoted, Eisenreich et al. 1981)
   0.045–0.07  (quoted literature range, Westcott et al. 1981)
   0.010–0.06  (quoted literature range, Mills et al. 1982)
   0.042  (quoted, Chou & Griffin 1986)
   0.035  (quoted, Eisenreich 1987)
   0.14  (selected, Mackay 1986; Metcalfe et al. 1988)
   0.043  (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   0.00107  (ebulliometry, Burrows 1946)
   0.00048  (20°C, Nisbet & Sarofim 1972)
   0.0103  (Monsanto 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
   log (Pₚ/mmHg) = 8.80 – 3700/(T/K) (temp range 150–300°C, from Monsanto 1972, NAS 1979)
   0.0103  (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Bidleman & Christinsen 1979 Giam et al. 1980; Westcott et al. 1980)
### Polychlorinated Biphenyls (PCBs)

**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):**

<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>279.7</td>
<td>(calculated, Mackay &amp; Leinonen 1975)</td>
</tr>
<tr>
<td>0.0993</td>
<td>(Murphy &amp; Rzeszutko 1977; quoted, Eisenreich et al. 1983)</td>
</tr>
<tr>
<td>273</td>
<td>(Slinn et al. 1978)</td>
</tr>
<tr>
<td>274</td>
<td>(calculated-P/C, Eisenreich et al. 1981)</td>
</tr>
<tr>
<td>0.007</td>
<td>(Eisenreich et al. 1981a)</td>
</tr>
<tr>
<td>0.0142</td>
<td>(Doskey &amp; Andren 1981; quoted, Eisenreich et al. 1983)</td>
</tr>
<tr>
<td>21.0</td>
<td>(direct concn. ratio-GC/ECD, Murphy et al. 1983)</td>
</tr>
<tr>
<td>28.67</td>
<td>(calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)</td>
</tr>
<tr>
<td>50.0</td>
<td>(calculated, Mackay et al. 1986)</td>
</tr>
<tr>
<td>18.24</td>
<td>(20°C, selected, Murphy et al. 1987 from Burkhard et al. 1985b)</td>
</tr>
<tr>
<td>19.25</td>
<td>(20°C, equilibrium concn. ratio, Murphy et al. 1987)</td>
</tr>
<tr>
<td>19.25</td>
<td>(20°C, selected from literature experimentally measured data, Staudinger &amp; Roberts 1996, 2001)</td>
</tr>
</tbody>
</table>

$\log K_{AW} = 11.880 - 4099/(T/K)$, (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

### Octanol/Water Partition Coefficient, $\log K_{ow}$:

- **6.03** (Hansch et al. 1973; Callahan et al. 1979; Mabey et al. 1982)
- **6.47** (GC-RT correlation, Veith et al. 1979b; Veith & Kosian 1983; quoted, Mackay 1982; Garten & Trabalka 1983; Zaroogian et al. 1985; Södergren 1987; Travis & Arms 1988)
- **6.72** (HPLC-RT correlation, Veith et al. 1979a)
- **4.08** (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
- **6.0** (quoted, Mills et al. 1982)
- **6.79** (literature mean, Di Toro et al. 1985)
- **6.1–6.8** (selected, Mackay et al. 1983, 1986; Metcalfe et al. 1988)
- **7.17** (Rapaport & Eisenreich 1984)
- **6.11** (quoted, Chou & Griffin 1986)
- **6.50** (quoted, Thomann 1989)

### Bioconcentration Factor, log $BCF$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source/Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.57</td>
<td>(spot fish, Hansen et al. 1971; quoted, Waid 1986)</td>
</tr>
<tr>
<td>4.85</td>
<td>(bluegill sunfish, Stalling &amp; Mayer 1972)</td>
</tr>
<tr>
<td>4.75–4.79</td>
<td>(channel catfish, Mayer et al. 1977; quoted, Waid 1986)</td>
</tr>
<tr>
<td>5.08, 5.57, 6.08</td>
<td>(Mysis, sculpins, pelagic fish, Veith et al. 1977)</td>
</tr>
<tr>
<td>5.00</td>
<td>(fathead minnow, 32-d exposure, Veith et al. 1979b; Veith &amp; Kosian 1983)</td>
</tr>
<tr>
<td>5.0–5.22, 4.41, 4.57</td>
<td>(oyster; shrimp, estuarine fish, Hansen et al. 1976; NAS 1979)</td>
</tr>
<tr>
<td>0.79, 0.78</td>
<td>(adipose tissue of male, female Albino rats, Geyer et al. 1980)</td>
</tr>
<tr>
<td>4.66, 4.08</td>
<td>(fish, flowing water, static water, Kenaga &amp; Goring 1980)</td>
</tr>
<tr>
<td>4.66</td>
<td>(quoted, Bysshe 1982)</td>
</tr>
<tr>
<td>5.12</td>
<td>(microorganism, calculated-$K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>5.00, 5.15</td>
<td>(fish: quoted, calculated-$K_{ow}$, Mackay 1982)</td>
</tr>
<tr>
<td>4.57</td>
<td>(fish, estuarine, Hansen et al. 1976; NAS 1979)</td>
</tr>
<tr>
<td>0.53, 4.70, 0.77, 0.79, 0.18, 0.98, 0.03</td>
<td>(cow, fish, poultry, rodents, sheep, small birds, swine, Garten &amp; Trabalka 1983)</td>
</tr>
</tbody>
</table>
5.69, 5.63; 6.11, 5.76 (live bacteria, dead bacteria; live algae, dead algae, Weber, Jr. et al. 1983)
5.0 (fathead minnow, quoted, Zaroogian et al. 1985)
4.80, 4.68 (oyster, quoted, Zaroogian et al. 1985)
4.8–5.51 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
5.52 (oyster, Södergren 1987)
−1.28, −1.95, −1.77 (beef, milk, vegetable, reported as biotransfer factor \( \log B_{b}, \log B_{m}, \log B_{v} \), Travis & Arms 1988)
4.95, 6.65 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.0, > 5.98 (fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor, \( \log BAF \):

7.21 (field data, lake trout-L/kg(Ip), Thomann 1989)
6.9, 6.51, 6.67, 6.8 (field data, large-mouth bass, L/kg(Ip), Thomann 1989)

Partition Coefficient, \( \log K_{p} \) or \( \log K_{d} \):

5.06, 4.95, 5.07 (suspended solids: Huron River, Saginaw River1, Saginaw River 2, Weber, Jr. et al. 1983)

Sorption Partition Coefficient, \( \log K_{OC} \):

6.0 (sediment/pore water 2.0% OC of pond, Halter & Johnson 1977; selected, Di Toro et al. 1985)
5.72 (sediment, calculated-KOW, Mabey et al. 1982)
5.44 (sediment/pore water 0.7–3.8% OC-Lake Michigan, Eadie et al. 1983; selected, Di Toro et al. 1985)
6.17, 6.16, 5.89 (clay: Montmorillonite 0.11% OC, natural Blue clay 1.82% OC, stripped Blue clay 0.47% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
5.84, 5.04, 6.31, 6.68, 6.29, 6.19, 6.34, 7.20 (sediments: Saginaw River 1. natural 3.45% OC, Saginaw River 1. stripped 1.05% OC, Saginaw R. 2. natural 2.61% OC, Saginaw River 2. NaOH ext. 1.98% OC, Saginaw River 2. benzene/MeOH ext. 1.84% OC, Saginaw River 2. stripped 0.67% OC, Saginaw River 2. < 75 µm 3.51% OC, Saignaw Bay 0.07% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
6.65 (suspended solids/subsurface water, 56% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.88 (sediment/pore water, 0.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.61 (sediment/pore water, 1.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.82 (sediment/pore water, 3.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
6.62 (calculated, Sklarew & Girvin 1987)
4.81 (soil, calculated-S, Chou & Griffin 1986)
6.02 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

Volatilization/Evaporation: volatilization rate \( k \sim 2 \times 10^{-6} \) g cm\(^{-2}\) d\(^{-1}\) at 26°C and \( k = 8.6 \times 10^{-5} \) g cm\(^{-2}\) d\(^{-1}\) at 60°C (Haque et al. 1974);
\( k = 0.10 \) µg m\(^{-2}\) d\(^{-1}\) with \( t_{1/2} = 28 \) d (Baker et al. 1985);
\( k = 2.7 \times 10^{-3} \) g m\(^{-2}\) h\(^{-1}\) (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant.
Polychlorinated Biphenyls (PCBs)

Oxidation: calculated rate constant for singlet oxygen, \( k << 360 \text{ M}^{-1} \text{ h}^{-1} \) and, \( k << 1 \text{ M}^{-1} \text{ h}^{-1} \) for \( \text{RO}_2 \) (peroxy radical) (Mabey et al. 1982).

Biodegradation: no reduction of concentration in the spilled transformer fluid contaminant of Aroclor was detected over a two-year period (Moein et al. 1976; quoted, Pal et al. 1980). 15.2% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972); 19% degraded by activated sludge for 48-h exposure (Callahan et al. 1979); biodegradation with a first-order \( k = 0.1 \text{ d}^{-1} \) by acclimated activated sludge and \( t_{1/2} = 7.0 \text{ d} \) (Callahan et al. 1979);
t aerobic biodegradation \( t_{1/2} = 81.9 \text{ d} \) without the addition of polymer chitin, \( t_{1/2} = 36.4 \text{ d} \) with chitin and \( t_{1/2} = 35.5 \text{ d} \) with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated \( k \sim 3 \times 10^{-9} \) to \( 3 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1} \) for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[
k_2 = 0.023 \text{ d}^{-1} \quad (0 \text{ to } 1 \text{ d}), \quad k_2 = 0.086 \text{ d}^{-1} \quad (1 \text{ to } 2 \text{ d}), \quad \text{and } k_2 = 0.0899 \text{ d}^{-1} \quad (2 \text{ to } 6 \text{ d}) \quad \text{with a biological }
\]
\[
t_{1/2} = 5.5 \text{ d} \quad \text{(mosquito larvae, Gooch & Hamdy 1982; selected, Waid 1986)}
\]
\[
k_2 = 0.131 \text{ d}^{-1}, \quad 0.137 \text{ d}^{-1} \quad \text{with biological } t_{1/2} = 4.7 \text{ d} \quad \text{(guppies, Gooch & Hamdy 1982; quoted, Waid 1986)}
\]
\[
k_2 = 0.102 \text{ d}^{-1} \quad \text{(first day)}, \quad k_2 = 0.057 \text{ d}^{-1} \quad \text{(thereafter)} \quad \text{with a biological } t_{1/2} = 6.1 \text{ d} \quad \text{(cichlids, Gooch & Hamdy 1982; quoted, Waid 1986)}
\]

Half-Lives in the Environment:

Air:
Surface water: volatilization \( t_{1/2} \sim 10 \text{ h} \) from 1 meter depth in 1 m³ water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:
Soil: volatilization \( t_{1/2} \sim 15 \text{ d} \) from an Ottawa sand (Haque et al. 1974; quoted, Pal et al. 1980);
\( t_{1/2} > 50 \text{ d} \) in soil (Ryan et al. 1988).

Biota: \( t_{1/2} < 12 \text{ d} \) in plant surface (Pal et al. 1980);
\( t_{1/2} = 3.3 \text{ d} \) in guppies, and \( t_{1/2} = 5.1 \text{ d} \) cichlids (Gooch & Hamdy 1982; quoted, Waid 1986).
### 7.1.3.7 Aroclor 1260

**Common Name:** Aroclor 1260  
**Synonym:**  
**Chemical Name:**  
**CAS Registry No:** 11096-82-5  
**Molecular Formula:**  
**Average Molecular Weight:** 372–375.7  
**Physical State:** sticky resin  
**Distillation Range (°C):**  
385–420 (NAS 1979; Brinkman & De Kock 1980)  
**Chlorine Content:** 60%  
**Density (g/cm³):**  
1.62 (20°C, Brinkman & De Kock 1980)  
1.55–1.56 (90°C, NAS 1979)  
1.58 (Callahan et al. 1979; Mills et al. 1982)  
1.60 (Mackay 1986; Metcalfe et al. 1988)  
**Molar Volume (cm³/mol):**  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**  
**Entropy of Fusion, ΔS_{fus} (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:**  
**Water Solubility (g/m³ or mg/L at 25°C):**  
0.025 (Monsanto 1972)  
0.025 (20°C, Nisbet & Sarofim 1972)  
0.0027 (Mackay & Wolkoff 1973; quoted, Callahan et al. 1979; Geyer et al. 1980; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Richardson et al. 1983; Chou & Griffin 1986)  
0.080 (shake flask-nephelometry, Hollifield 1979)  
0.003 (quoted, Brinkman & De Kock 1980; Mackay et al. 1983; Eisenreich 1987)  
0.0144 (20°C, calculated-mole fraction, Murphy et al. 1987)  
**Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):**  
2.67 × 10⁻⁵ (38°C, Nisbet & Sarofim 1972)  
0.0054 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983)  
0.012 (20°C, extrapolated, Monsanto 1972; NAS 1979)  
log (P$_\text{mm Hg}$/T/K) = 8.50 – 3700/T(K) (temp range 150–300°C, from Monsanto 1972, NAS 1979)  
0.0054 (Callahan et al. 1979; Mabey et al. 1982; Richardson et al. 1983)  
0.0053 (Pal et al. 1980; Mills et al. 1982)  
0.0004 (38°C, average, Wingender & Williams 1984)  
0.00183, 0.00162 (GC-RT, Foreman & Bidleman 1985)  
0.003 (quoted, Erickson 1986)  
0.00064 (Mackay 1986; Metcalfe et al. 1988)  
0.000284 (quoted, Eisenreich 1987)  
0.000841 (20°C, calculated-mole fraction, Murphy et al. 1987)  
**Henry’s Law Constant (Pa m³/mol):**  
722.4 (calculated, Mackay & Leinonen 1975)  
718 (Slinn et al. 1978)  
719 (quoted, Mills et al. 1982)  
88.0 (suggested, Mackay et al. 1983)  
72.24 (16°C, calculated-P/C, Richardson et al. 1983)  
34.04 (calculated, Burkhardt et al. 1985b; quoted, Eisenreich 1987)  
21.27 (20°C, quoted, Murphy et al. 1987 from Burkhardt et al. 1985b)
Polychlorinated Biphenyls (PCBs)

17.23 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
17.23 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log $K_{aw} = 11.848 - 4104/(T/K)$ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $log K_{ow}$:

7.14 (Chiou et al. 1977)
6.11 (Chiou et al. 1977; Callahan et al. 1979; quoted, Ryan et al. 1988)
7.15 (Callahan et al. 1979; Mabey et al. 1982)
6.91 (GC-RT correlation, Veith et al. 1979a; Veith & Kosian 1983; quoted, Mackay 1982; Geyer et al. 1987)
4.34 (Pal et al. 1980)
> 6.0 (quoted, Mills et al. 1982)
6.30–7.50 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
6.61 (calculated-S, Chou & Griffin 1986)
6.90 (quoted, Thomann 1989)

Bioconcentration Factor, $log BCF$:

5.43 (fathead minnows, DeFoe et al. 1978; quoted, Waid 1986)
5.29 (fathead minnow, 32-d exposure, Veith et al. 1979a; Veith & Kosian 1983)
0.672 (adipose tissue of male albino rats, Geyer et al. 1980)
5.29, 5.59 (fish: quoted, calculated-$K_{ow}$, Mackay 1982)
6.11 (microorganism, calculated-$K_{ow}$, Mabey et al. 1982)
5.0–6.20 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
2.28–2.50 (human fat of lipid basis, calculated-$K_{ow}$, Geyer et al. 1987)
2.11–2.36 (human fat of wet wt. basis, calculated-$K_{ow}$, Geyer et al. 1987)
4.38 ($Rhabdosargus holubi$, De Kock & Lord 1988)
4.80, 6.72 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.22, 6.50 (fathead minnow, male, 250-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.43, 6.53 (fathead minnow, female, 250-d uptake, wet wt basis, lipid wt basis, Geyer et al. 2000)
2.24, 2.40 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $log K_{oc}$:

6.83 (sediment, calculated-$K_{ow}$, Mabey et al. 1982)
5.54 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volutilization/Evaporation: estimated evaporation rate from liquid surfaces at 100°C to be 0.009 mg/cm²·h (Hutzinger et al. 1974);
$t_\frac{1}{2} \approx 7.53$ h of evaporation from water depth of 1 m (Mackay & Leinonen 1975)
rate of evaporation $k = 2.9 \times 10^{-4}$ g m⁻²·h⁻¹ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:
Hydrolysis: not environmentally significant (Mabey et al. 1982).
Oxidation: calculated rate constant for singlet oxygen, $k << 360$ M⁻¹·h⁻¹ and $k << 1$ M⁻¹·h⁻¹ for RO₂ (peroxy radical) (Mabey et al. 1982).
Biotransformation: $k \approx 3 \times 10^{-4}$ to $3 \times 10^{-12}$ mL·cell⁻¹·h⁻¹, transformation for bacteria in water (Mabey et al. 1982)
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 332$ d⁻¹; $k_2 = 0.014$ d⁻¹ ($Rhabdosargus holubi$, De Kock & Lord 1988)
log $k_2 = -2.40$ d⁻¹ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:
Air:
Surface water: volatilization $t_{1/2} \sim 10$ h at 1 m depth of 1 m$^3$ of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).
River water: volatilization $t_{1/2} \sim 52$ d (Oloffs et al. 1972; selected, Pal et al. 1980).

Sediment:

Soil:

Biota: $t_{1/2} = 50$ d in *Rhabdosargus holubi* (De Kock & Lord 1988).
## 7.2 SUMMARY TABLES AND QSPR PLOTS

### TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Biphenyl</td>
<td>92-52-4</td>
<td>154.207</td>
<td>68.93</td>
<td>256.1</td>
<td>0.371</td>
<td>184.6</td>
</tr>
<tr>
<td>1</td>
<td>2-</td>
<td>2051-60-7</td>
<td>188.652</td>
<td>34</td>
<td>274</td>
<td>0.816</td>
<td>205.5</td>
</tr>
<tr>
<td>2</td>
<td>3-</td>
<td>2051-61-8</td>
<td>188.652</td>
<td>16</td>
<td>284.5</td>
<td>1</td>
<td>205.5</td>
</tr>
<tr>
<td>3</td>
<td>4-</td>
<td>2051-62-9</td>
<td>188.652</td>
<td>78.8</td>
<td>292.9</td>
<td>0.297</td>
<td>205.5</td>
</tr>
<tr>
<td>4</td>
<td>2,2′-</td>
<td>13029-08-8</td>
<td>223.098</td>
<td>60.5</td>
<td></td>
<td>0.448</td>
<td>226.4</td>
</tr>
<tr>
<td>5</td>
<td>2,3-</td>
<td>16605-91-7</td>
<td>223.098</td>
<td>28</td>
<td></td>
<td>0.934</td>
<td>226.4</td>
</tr>
<tr>
<td>6</td>
<td>2,3′</td>
<td>25569-80-6</td>
<td>223.098</td>
<td></td>
<td></td>
<td></td>
<td>226.4</td>
</tr>
<tr>
<td>7</td>
<td>2,4-</td>
<td>33284-50-3</td>
<td>223.098</td>
<td>24.4</td>
<td></td>
<td>1</td>
<td>226.4</td>
</tr>
<tr>
<td>8</td>
<td>2,4′-</td>
<td>34883-43-7</td>
<td>223.098</td>
<td>43</td>
<td></td>
<td>0.666</td>
<td>226.4</td>
</tr>
<tr>
<td>9</td>
<td>2,5-</td>
<td>34883-39-1</td>
<td>223.098</td>
<td>22–23</td>
<td></td>
<td>1</td>
<td>226.4</td>
</tr>
<tr>
<td>10</td>
<td>2,6-</td>
<td>33146-45-1</td>
<td>223.098</td>
<td>35.5</td>
<td></td>
<td>0.789</td>
<td>226.4</td>
</tr>
<tr>
<td>11</td>
<td>3,3′-</td>
<td>2050-67-1</td>
<td>223.098</td>
<td>29</td>
<td>320</td>
<td>0.914</td>
<td>226.4</td>
</tr>
<tr>
<td>12</td>
<td>3,4-</td>
<td>2974-92-7</td>
<td>223.098</td>
<td>49</td>
<td>195–200</td>
<td>0.581</td>
<td>226.4</td>
</tr>
<tr>
<td>13</td>
<td>3,4′-</td>
<td>2974-90-5</td>
<td>223.098</td>
<td></td>
<td></td>
<td></td>
<td>226.4</td>
</tr>
<tr>
<td>14</td>
<td>3,5-</td>
<td>34883-41-5</td>
<td>223.098</td>
<td>31</td>
<td></td>
<td>0.873</td>
<td>226.4</td>
</tr>
<tr>
<td>15</td>
<td>4,4′-</td>
<td>2050-68-2</td>
<td>223.098</td>
<td>149.3</td>
<td>317</td>
<td>0.0603</td>
<td>226.4</td>
</tr>
<tr>
<td>16</td>
<td>2,2′,3-</td>
<td>38444-78-9</td>
<td>257.543</td>
<td>28</td>
<td></td>
<td>0.934</td>
<td>247.3</td>
</tr>
<tr>
<td>17</td>
<td>2,2′,4-</td>
<td>37680-66-3</td>
<td>257.543</td>
<td></td>
<td></td>
<td></td>
<td>247.3</td>
</tr>
<tr>
<td>18</td>
<td>2,2′,5-</td>
<td>37680-65-2</td>
<td>257.543</td>
<td>44</td>
<td></td>
<td>0.651</td>
<td>247.3</td>
</tr>
<tr>
<td>19</td>
<td>2,2′,6-</td>
<td>38444-73-4</td>
<td>257.543</td>
<td></td>
<td></td>
<td></td>
<td>247.3</td>
</tr>
<tr>
<td>20</td>
<td>2,3,3′-</td>
<td>38444-84-7</td>
<td>257.543</td>
<td></td>
<td></td>
<td></td>
<td>247.3</td>
</tr>
<tr>
<td>21</td>
<td>2,3,4-</td>
<td>55702-46-0</td>
<td>257.543</td>
<td>102</td>
<td></td>
<td>0.176</td>
<td>247.3</td>
</tr>
<tr>
<td>22</td>
<td>2,3,4′-</td>
<td>38444-85-8</td>
<td>257.543</td>
<td>73</td>
<td></td>
<td>0.338</td>
<td>247.3</td>
</tr>
<tr>
<td>23</td>
<td>2,3,5-</td>
<td>55720-44-0</td>
<td>257.543</td>
<td>41</td>
<td></td>
<td>0.697</td>
<td>247.3</td>
</tr>
<tr>
<td>24</td>
<td>2,3,6-</td>
<td>55702-45-9</td>
<td>257.543</td>
<td>49</td>
<td></td>
<td>0.581</td>
<td>247.3</td>
</tr>
<tr>
<td>25</td>
<td>2,3′,4-</td>
<td>55712-37-3</td>
<td>257.543</td>
<td></td>
<td></td>
<td></td>
<td>247.3</td>
</tr>
<tr>
<td>26</td>
<td>2,3′,5-</td>
<td>38444-81-4</td>
<td>257.543</td>
<td>40.5</td>
<td></td>
<td>0.705</td>
<td>247.3</td>
</tr>
<tr>
<td>27</td>
<td>2,3′,6-</td>
<td>38444-76-7</td>
<td>257.543</td>
<td></td>
<td></td>
<td></td>
<td>247.3</td>
</tr>
<tr>
<td>28</td>
<td>2,4,4′-</td>
<td>7012-37-5</td>
<td>257.543</td>
<td>57</td>
<td></td>
<td>0.485</td>
<td>247.3</td>
</tr>
<tr>
<td>29</td>
<td>2,4,5-</td>
<td>15862-07-4</td>
<td>257.543</td>
<td>78.5</td>
<td></td>
<td>0.299</td>
<td>247.3</td>
</tr>
</tbody>
</table>
### TABLE 7.2.1 (Continued)
Summary of physical-chemical properties of some PCB congeners

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>2,4,6-</td>
<td>35693-92-6</td>
<td>257.543</td>
<td>62.5</td>
<td></td>
<td>0.429</td>
<td>247.3</td>
</tr>
<tr>
<td>31</td>
<td>2,4',5-</td>
<td>16606-02-3</td>
<td>257.543</td>
<td>67</td>
<td></td>
<td>0.387</td>
<td>247.3</td>
</tr>
<tr>
<td>32</td>
<td>2,4'6-</td>
<td>38444-77-8</td>
<td>257.543</td>
<td></td>
<td></td>
<td>0.454</td>
<td>247.3</td>
</tr>
<tr>
<td>33</td>
<td>2,3',4'-</td>
<td>38444-86-9</td>
<td>257.543</td>
<td>60</td>
<td></td>
<td>0.474</td>
<td>247.3</td>
</tr>
<tr>
<td>34</td>
<td>2,3',5'-</td>
<td>37680-68-5</td>
<td>257.543</td>
<td>58</td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>35</td>
<td>3,3'-4'</td>
<td>37680-69-6</td>
<td>257.543</td>
<td>87</td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>36</td>
<td>3,3'-5'</td>
<td>38444-87-0</td>
<td>257.543</td>
<td></td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>37</td>
<td>3,4',4'-</td>
<td>38444-90-5</td>
<td>257.543</td>
<td>87</td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>38</td>
<td>3,4'-</td>
<td>53555-66-1</td>
<td>257.543</td>
<td></td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>39</td>
<td>3,4',5'-</td>
<td>38444-88-1</td>
<td>257.543</td>
<td>88</td>
<td></td>
<td>0.246</td>
<td>247.3</td>
</tr>
<tr>
<td>40</td>
<td>2',2'3',3'-'</td>
<td>38444-93-8</td>
<td>291.988</td>
<td>121</td>
<td></td>
<td>0.114</td>
<td>268.2</td>
</tr>
<tr>
<td>41</td>
<td>2',2'3',4'-'</td>
<td>52663-59-9</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.114</td>
<td>268.2</td>
</tr>
<tr>
<td>42</td>
<td>2',2'3',4'-'</td>
<td>36559-22-5</td>
<td>291.988</td>
<td>69</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>43</td>
<td>2',2'3',5'-'</td>
<td>70362-46-8</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>44</td>
<td>2',2'3',5'-'</td>
<td>41464-39-5</td>
<td>291.988</td>
<td>47</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>45</td>
<td>2',2'3',6'-'</td>
<td>70362-45-7</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>46</td>
<td>2',2'3',6'-'</td>
<td>41464-47-5</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>47</td>
<td>2',2'4',4'-'</td>
<td>2437-79-8</td>
<td>291.988</td>
<td>83</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>48</td>
<td>2',2'4',5'-'</td>
<td>70362-47-9</td>
<td>291.988</td>
<td>65.9</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>49</td>
<td>2',2'4',5'-'</td>
<td>41464-40-8</td>
<td>291.988</td>
<td>66.5</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>50</td>
<td>2',2'4',6'-'</td>
<td>62796-65-8</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>51</td>
<td>2',2'4',6'-'</td>
<td>68194-04-7</td>
<td>291.988</td>
<td>66</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>52</td>
<td>2',2'5',5'-'</td>
<td>35693-99-3</td>
<td>291.988</td>
<td>87</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>53</td>
<td>2',2'5',6'-'</td>
<td>41464-41-9</td>
<td>291.988</td>
<td>104</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>54</td>
<td>2',2'6',6'-'</td>
<td>15968-05-5</td>
<td>291.988</td>
<td>198</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>55</td>
<td>2',3',3',4'-'</td>
<td>74338-24-2</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>56</td>
<td>2',3',3',4'-'</td>
<td>41464-43-1</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>57</td>
<td>2',3',3',5'-'</td>
<td>70424-67-8</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>58</td>
<td>2',3',3',5'-'</td>
<td>41464-49-7</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>59</td>
<td>2',3',3',6'-'</td>
<td>74472-33-6</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>60</td>
<td>2',3',4',4'-'</td>
<td>33025-41-1</td>
<td>291.988</td>
<td>142</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>61</td>
<td>2',3',4',5'-'</td>
<td>33284-53-6</td>
<td>291.988</td>
<td>92.2</td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td>62</td>
<td>2',3',4',6'-'</td>
<td>54230-23-7</td>
<td>291.988</td>
<td></td>
<td></td>
<td>0.370</td>
<td>268.2</td>
</tr>
<tr>
<td></td>
<td>Formula</td>
<td>CAS Number</td>
<td>Molecular Weight</td>
<td>Pesticide</td>
<td>Enzyme Concentration</td>
<td>Acetylcholinesterase Inhibition</td>
<td>Butyrylcholinesterase Inhibition</td>
</tr>
<tr>
<td>---</td>
<td>---------</td>
<td>------------</td>
<td>------------------</td>
<td>------------</td>
<td>----------------------</td>
<td>-------------------------------</td>
<td>--------------------------------</td>
</tr>
<tr>
<td>63</td>
<td>2,3,4',5-</td>
<td>74472–34–7</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>2,3,4'-6-</td>
<td>52663–58–8</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>2,3,5,6-</td>
<td>33284-54-7</td>
<td>291.988</td>
<td></td>
<td>79</td>
<td>0.295</td>
<td></td>
</tr>
<tr>
<td>66</td>
<td>2,3',4'-</td>
<td>32598-10-0</td>
<td>291.988</td>
<td></td>
<td>124</td>
<td>0.107</td>
<td></td>
</tr>
<tr>
<td>67</td>
<td>2,3',4'-5-</td>
<td>73575–53–8</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>68</td>
<td>2,3',4'-6-</td>
<td>73575–52–7</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>69</td>
<td>2,3',4-</td>
<td>60233–24–1</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>2,3',5-</td>
<td>32598-11-1</td>
<td>291.988</td>
<td></td>
<td>104</td>
<td>0.168</td>
<td></td>
</tr>
<tr>
<td>71</td>
<td>2,3',6-</td>
<td>41464–46–4</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>72</td>
<td>2,4',5-</td>
<td>41464–42–0</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>73</td>
<td>2,4',6-</td>
<td>74338–23–1</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>74</td>
<td>2,4',5'</td>
<td>32690–93–0</td>
<td>291.988</td>
<td></td>
<td>125</td>
<td>0.104</td>
<td></td>
</tr>
<tr>
<td>75</td>
<td>2,4',6'</td>
<td>32598-12-2</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>76</td>
<td>2,3',4',5'</td>
<td>70362-48-0</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>77</td>
<td>3,3',4',4'</td>
<td>32598-13-3</td>
<td>291.988</td>
<td></td>
<td>180</td>
<td>0.0301</td>
<td></td>
</tr>
<tr>
<td>78</td>
<td>3,3',4',5'</td>
<td>70362–49–1</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>79</td>
<td>3,3',4',5'</td>
<td>41464–48–6</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>3,3',5',5'</td>
<td>33284-52-5</td>
<td>291.988</td>
<td></td>
<td>164</td>
<td>0.0433</td>
<td></td>
</tr>
<tr>
<td>81</td>
<td>3,4',4',5'</td>
<td>70362–50–4</td>
<td>291.988</td>
<td></td>
<td></td>
<td>268.2</td>
<td></td>
</tr>
<tr>
<td>82</td>
<td>2,2',3,3',4'</td>
<td>52663–62–4</td>
<td>326.433</td>
<td></td>
<td>65</td>
<td>0.405</td>
<td></td>
</tr>
<tr>
<td>83</td>
<td>2,2',3,3',5'</td>
<td>60145-20-2</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>84</td>
<td>2,2',3,3',6'</td>
<td>52663–60-2</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>2,2',3,4',4'</td>
<td>65510-45-4</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>86</td>
<td>2,2',3,4',5'</td>
<td>55312-69-1</td>
<td>326.433</td>
<td></td>
<td>100</td>
<td>0.184</td>
<td></td>
</tr>
<tr>
<td>87</td>
<td>2,2',3,4',5'</td>
<td>38380-02-8</td>
<td>326.433</td>
<td></td>
<td>114</td>
<td>0.134</td>
<td></td>
</tr>
<tr>
<td>88</td>
<td>2,2',3,4',6'</td>
<td>55215-17-3</td>
<td>326.433</td>
<td></td>
<td>100</td>
<td>0.184</td>
<td></td>
</tr>
<tr>
<td>89</td>
<td>2,2',3,4',6'</td>
<td>73575–57–2</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>2,2',3,4',5'</td>
<td>68194–07-0</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>91</td>
<td>2,2',3,4',6'</td>
<td>58194–05-8</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>92</td>
<td>2,2',3,5',5'</td>
<td>52663–61-3</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>2,2',3,5',6'</td>
<td>73575–56–1</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>94</td>
<td>2,2',3,5',6'</td>
<td>73575–55-0</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>95</td>
<td>2,2',3,5',6'</td>
<td>38379-99-6</td>
<td>326.433</td>
<td></td>
<td>100</td>
<td>0.184</td>
<td></td>
</tr>
<tr>
<td>96</td>
<td>2,2',3,6',6'</td>
<td>73575–54-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>97</td>
<td>2,2',3,4',5'</td>
<td>41464–51–1</td>
<td>326.433</td>
<td></td>
<td>82</td>
<td>0.276</td>
<td></td>
</tr>
<tr>
<td>98</td>
<td>2,2',3,4',6'</td>
<td>60233–25-2</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
<tr>
<td>99</td>
<td>2,2',4',4',5'</td>
<td>38380-01-7</td>
<td>326.433</td>
<td></td>
<td></td>
<td>289.1</td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th>IUPAC no.</th>
<th>Congener</th>
<th>CAS no.</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Le Bas molar volume, V_m (cm³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>2,2′,4,4′,6-</td>
<td>39485-83-1</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>101</td>
<td>2,2′,4,5,5′-</td>
<td>37680-73-2</td>
<td>326.433</td>
<td></td>
<td>78.5</td>
<td>0.299</td>
<td>289.1</td>
</tr>
<tr>
<td>102</td>
<td>2,2′,4,5,6′-</td>
<td>68194-06-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>103</td>
<td>2,2′,4,5,6′-</td>
<td>60145-21-3</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>104</td>
<td>2,2′,4,6,6′-</td>
<td>56558-16-8</td>
<td>326.433</td>
<td></td>
<td>85</td>
<td>0.258</td>
<td>289.1</td>
</tr>
<tr>
<td>105</td>
<td>2,3,3′,4,4′-</td>
<td>32598-14-4</td>
<td>326.433</td>
<td></td>
<td>105</td>
<td>0.164</td>
<td>289.1</td>
</tr>
<tr>
<td>106</td>
<td>2,3,3′,4,5-</td>
<td>70424-69-0</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>107</td>
<td>2,3,3′,4,5′-</td>
<td>70424-68-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>108</td>
<td>2,3,3′,4,6′-</td>
<td>70362-41-3</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>109</td>
<td>2,3,3′,4,6′-</td>
<td>74472-35-8</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>110</td>
<td>2,3,3′,4,6′-</td>
<td>38380-03-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>111</td>
<td>2,3,3′,5,5′-</td>
<td>39635-32-0</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>112</td>
<td>2,3,3′,5,6′-</td>
<td>74472-36-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>113</td>
<td>2,3,3′,5,6′-</td>
<td>68194-10-5</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>114</td>
<td>2,3,4,4′-</td>
<td>74472-37-0</td>
<td>326.433</td>
<td></td>
<td>99</td>
<td>0.188</td>
<td>289.1</td>
</tr>
<tr>
<td>115</td>
<td>2,3,4,4′,5′-</td>
<td>74472-38-1</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>116</td>
<td>2,3,4,5,6′-</td>
<td>18259-05-7</td>
<td>326.433</td>
<td></td>
<td>123.5</td>
<td>0.108</td>
<td>289.1</td>
</tr>
<tr>
<td>117</td>
<td>2,3,4,5,6′-</td>
<td>68194-11-6</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>118</td>
<td>2,3,4,5′,6′-</td>
<td>31508-00-6</td>
<td>326.433</td>
<td></td>
<td>107</td>
<td>0.157</td>
<td>289.1</td>
</tr>
<tr>
<td>119</td>
<td>2,3,4,5′,6′-</td>
<td>56558-17-9</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>120</td>
<td>2,3,4,5′,5′-</td>
<td>68194-12-7</td>
<td>326.433</td>
<td></td>
<td>77</td>
<td>0.309</td>
<td>289.1</td>
</tr>
<tr>
<td>121</td>
<td>2,3,4,5′,6′-</td>
<td>56558-18-0</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>122</td>
<td>2,3,4,5′,5′-</td>
<td>76842-07-4</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>123</td>
<td>2,3,4,5′,5′-</td>
<td>65510-44-3</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>124</td>
<td>2,3,4′,5′-</td>
<td>70424-70-3</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>125</td>
<td>2,3,4′,5′,6′-</td>
<td>74472-39-2</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>126</td>
<td>3,3′,4,4′,5′-</td>
<td>57465-28-8</td>
<td>326.433</td>
<td></td>
<td>106</td>
<td>0.160</td>
<td>289.1</td>
</tr>
<tr>
<td>127</td>
<td>3′,3′,4,5′,5′-</td>
<td>39635-33-1</td>
<td>326.433</td>
<td></td>
<td></td>
<td></td>
<td>289.1</td>
</tr>
<tr>
<td>128</td>
<td>2,2′,3,3′,4,4′-</td>
<td>38380-07-3</td>
<td>360.878</td>
<td></td>
<td>151</td>
<td>0.058</td>
<td>310.0</td>
</tr>
<tr>
<td>129</td>
<td>2,2′,3,3′,4,5′-</td>
<td>55215-18-4</td>
<td>360.878</td>
<td></td>
<td>85</td>
<td>0.258</td>
<td>310.0</td>
</tr>
<tr>
<td>130</td>
<td>2,2′,3,3′,4,5′-</td>
<td>52663-66-8</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td>310.0</td>
</tr>
<tr>
<td>131</td>
<td>2,2′,3,3′,4,6′-</td>
<td>61798-70-7</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td>310.0</td>
</tr>
<tr>
<td>132</td>
<td>2,2′,3,3′,4,6′-</td>
<td>38380-05-1</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td>310.0</td>
</tr>
<tr>
<td>No.</td>
<td>Formula</td>
<td>CAS Number</td>
<td>Molecular Weight</td>
<td>Relative Molecular Weight</td>
<td>Vapors</td>
<td>Temp.</td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>---------</td>
<td>------------</td>
<td>------------------</td>
<td>--------------------------</td>
<td>--------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>133</td>
<td>2,2',3,3',5,5'-</td>
<td>35694-04-3</td>
<td>360.878</td>
<td>129</td>
<td>0.0954</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>134</td>
<td>2,2',3,3',5,6'-</td>
<td>52704-70-8</td>
<td>360.878</td>
<td>100</td>
<td>0.184</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>135</td>
<td>2,2',3,3',6,6'-</td>
<td>5274-13-5</td>
<td>360.878</td>
<td>310.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>136</td>
<td>2,2',3,4,4',5'-</td>
<td>38411-22-2</td>
<td>360.878</td>
<td>114.2</td>
<td>0.133</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>137</td>
<td>2,2',3,4,4',6'-</td>
<td>35694-06-5</td>
<td>360.878</td>
<td>78</td>
<td>0.302</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>138</td>
<td>2,2',3,4,4',7'-</td>
<td>35065-28-2</td>
<td>360.878</td>
<td>80</td>
<td>0.289</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>139</td>
<td>2,2',3,4,4',8'-</td>
<td>59291-64-4</td>
<td>360.878</td>
<td>310.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>2,2',3,4,5,5'-</td>
<td>52712-04-6</td>
<td>360.878</td>
<td>85</td>
<td>0.258</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>141</td>
<td>2,2',3,4,5,6'-</td>
<td>41411-61-4</td>
<td>360.878</td>
<td>136</td>
<td>0.0815</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>142</td>
<td>2,2',3,4,5,7'-</td>
<td>68194-15-0</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>143</td>
<td>2,2',3,4,6,6'-</td>
<td>68194-14-9</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>144</td>
<td>2,2',3,4,6,7'-</td>
<td>74472-40-5</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>145</td>
<td>2,2',3,4,8,6'-</td>
<td>74472-16-8</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>146</td>
<td>2,2',3,4,9,6'-</td>
<td>74472-17-9</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>147</td>
<td>2,2',3,5,5,6'-</td>
<td>38380-04-0</td>
<td>360.878</td>
<td>Oil</td>
<td>1</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>148</td>
<td>2,2',3,5,6,6'-</td>
<td>68194-08-1</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>149</td>
<td>2,2',3,5,6,7'-</td>
<td>52663-63-5</td>
<td>360.878</td>
<td>101</td>
<td>0.180</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>150</td>
<td>2,2',3,5,6,8'-</td>
<td>68194-09-2</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>151</td>
<td>2,2',3,5,7,7'-</td>
<td>35065-27-1</td>
<td>360.878</td>
<td>103.5</td>
<td>0.170</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>152</td>
<td>2,2',3,5,8,8'-</td>
<td>60145-22-4</td>
<td>360.878</td>
<td>Oil</td>
<td>1</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>153</td>
<td>2,2',3,5,9,8'-</td>
<td>33979-03-2</td>
<td>360.878</td>
<td>112.5</td>
<td>0.139</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>154</td>
<td>2,2',3,5,10,8'-</td>
<td>33830-08-4</td>
<td>360.878</td>
<td>127</td>
<td>0.100</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>155</td>
<td>2,2',3,6,6'-</td>
<td>69782-90-7</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>156</td>
<td>2,2',3,6,7,7'-</td>
<td>74472-42-7</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>157</td>
<td>2,2',3,6,8,8'-</td>
<td>74472-42-7</td>
<td>360.878</td>
<td>107</td>
<td>0.157</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>158</td>
<td>2,2',3,6,9,8'-</td>
<td>74635-35-3</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>159</td>
<td>2,2',3,6,10,8'-</td>
<td>41411-62-5</td>
<td>360.878</td>
<td>99</td>
<td>0.188</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>160</td>
<td>2,2',3,7,7,8'-</td>
<td>74472-43-8</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>161</td>
<td>2,2',3,7,8,8'-</td>
<td>39635-34-2</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>162</td>
<td>2,2',3,7,9,8'-</td>
<td>74472-44-9</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>163</td>
<td>2,2',3,7,10,8'-</td>
<td>74472-45-0</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>164</td>
<td>2,2',3,8,8,9'-</td>
<td>74472-46-1</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>165</td>
<td>2,2',3,8,9,10,8'-</td>
<td>74472-47-2</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>166</td>
<td>2,2',3,9,9,10,8'-</td>
<td>74472-48-3</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>167</td>
<td>2,2',4,4,5,5'-</td>
<td>41411-63-6</td>
<td>360.878</td>
<td>163</td>
<td>0.0433</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>168</td>
<td>2,2',4,4,5,6,6'-</td>
<td>52663-72-6</td>
<td>360.878</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>169</td>
<td>2,2',4,4,5,5,6'-</td>
<td>59291-65-5</td>
<td>360.878</td>
<td>110–111</td>
<td>0.145</td>
<td>310.0</td>
<td></td>
</tr>
<tr>
<td>170</td>
<td>2,2',4,4,4,5,5'-</td>
<td>35065-30-6</td>
<td>360.878</td>
<td>135</td>
<td>0.0833</td>
<td>330.0</td>
<td></td>
</tr>
</tbody>
</table>

(Continued)
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>171</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–71–5</td>
<td>395.323</td>
<td>117.5</td>
<td></td>
<td>0.124</td>
<td>330.9</td>
</tr>
<tr>
<td>172</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–74–8</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>173</td>
<td>2,2′,3′,4′,6′-</td>
<td>68194–16–1</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>174</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>38411–25–5</td>
<td>395.323</td>
<td>130.6</td>
<td></td>
<td>0.0920</td>
<td>330.9</td>
</tr>
<tr>
<td>175</td>
<td>2,2′,3′,4′,6′-</td>
<td>40186–70–7</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>176</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–65–7</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>177</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–70–4</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>178</td>
<td>2,2′,3′,5′,5′,6′-</td>
<td>52663–67–9</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>179</td>
<td>2,2′,3′,5′,6′-</td>
<td>52663–64–6</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>2,2′,3′,4′,5′,5′-</td>
<td>35065–29–3</td>
<td>395.323</td>
<td>110</td>
<td></td>
<td>0.147</td>
<td>330.9</td>
</tr>
<tr>
<td>181</td>
<td>2,2′,3′,4′,5′,5′-</td>
<td>74472–47–2</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>182</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>60145–23–5</td>
<td>395.323</td>
<td>152</td>
<td></td>
<td>0.0567</td>
<td>330.9</td>
</tr>
<tr>
<td>183</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–69–1</td>
<td>395.323</td>
<td>83</td>
<td></td>
<td>0.270</td>
<td>330.9</td>
</tr>
<tr>
<td>184</td>
<td>2,2′,3′,4′,6′,6′-</td>
<td>74472–48–3</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>185</td>
<td>2,2′,3′,4′,6′,6′-</td>
<td>52712–05–7</td>
<td>395.323</td>
<td>149</td>
<td></td>
<td>0.0607</td>
<td>330.9</td>
</tr>
<tr>
<td>186</td>
<td>2,2′,3′,5′,6′,6′-</td>
<td>74472–49–4</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>187</td>
<td>2,2′,3′,5′,6′,6′-</td>
<td>52663–68–0</td>
<td>395.323</td>
<td>149</td>
<td></td>
<td>0.0607</td>
<td>330.9</td>
</tr>
<tr>
<td>188</td>
<td>2,2′,3′,5′,6′,6′-</td>
<td>74487–85–7</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>189</td>
<td>2,3′,4′,4′,5′,6′-</td>
<td>39635–31–9</td>
<td>395.323</td>
<td>170</td>
<td></td>
<td>0.0378</td>
<td>330.9</td>
</tr>
<tr>
<td>190</td>
<td>2,3′,4′,4′,5′,6′-</td>
<td>41411–64–7</td>
<td>395.323</td>
<td>117</td>
<td></td>
<td>0.125</td>
<td>330.9</td>
</tr>
<tr>
<td>191</td>
<td>2,3′,4′,4′,5′,6′-</td>
<td>74472–50–7</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>192</td>
<td>2,3′,4′,5′,6′-</td>
<td>74472–51–8</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>193</td>
<td>2,3′,4′,5′,6′-</td>
<td>69782–91–8</td>
<td>395.323</td>
<td></td>
<td></td>
<td>330.9</td>
<td></td>
</tr>
<tr>
<td>194</td>
<td>2,2′,3′,4′,5′,5′,6′-</td>
<td>35694–08–7</td>
<td>429.768</td>
<td>159</td>
<td></td>
<td>0.0484</td>
<td>351.8</td>
</tr>
<tr>
<td>195</td>
<td>2,2′,3′,4′,5′,5′,6′-</td>
<td>52663–78–2</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>196</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>42740–50–1</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>197</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>33091–17–7</td>
<td>429.768</td>
<td>132</td>
<td></td>
<td>0.0892</td>
<td>351.8</td>
</tr>
<tr>
<td>198</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>68194–17–2</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td>1.759</td>
</tr>
<tr>
<td>199</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–75–9</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>52663–73–7</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>201</td>
<td>2,2′,3′,4′,5′,6′-</td>
<td>40186–71–8</td>
<td>429.768</td>
<td></td>
<td></td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>No.</td>
<td>Formula</td>
<td>CAS Number</td>
<td>Molecular Weight</td>
<td>T L</td>
<td>∆H</td>
<td>T L</td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>-------------------------</td>
<td>------------</td>
<td>------------------</td>
<td>-----</td>
<td>----</td>
<td>-----</td>
<td></td>
</tr>
<tr>
<td>202</td>
<td>2,2',3,3',5,5',6,6'</td>
<td>2136-99-4</td>
<td>429.768</td>
<td>161</td>
<td>0.0463</td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>203</td>
<td>2,2',3,4,4',5,5',6</td>
<td>52663-76-0</td>
<td>429.768</td>
<td>161</td>
<td>0.0463</td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>204</td>
<td>2,2',3,4,4',5,6,6'</td>
<td>74472-52-9</td>
<td>429.768</td>
<td>161</td>
<td>0.0463</td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>205</td>
<td>2,3,3',4,4',5,5',6</td>
<td>74472-53-0</td>
<td>429.768</td>
<td>161</td>
<td>0.0463</td>
<td>351.8</td>
<td></td>
</tr>
<tr>
<td>206</td>
<td>2,2',3,3',4,4',5,5',6</td>
<td>40186-72-9</td>
<td>464.213</td>
<td>206</td>
<td>0.0168</td>
<td>372.7</td>
<td></td>
</tr>
<tr>
<td>207</td>
<td>2,2',3,3',4,4',5,6,6'</td>
<td>52663-79-3</td>
<td>464.213</td>
<td>206</td>
<td>0.0168</td>
<td>372.7</td>
<td></td>
</tr>
<tr>
<td>208</td>
<td>2,2',3,3',4,5,5',6,6'</td>
<td>52663-77-1</td>
<td>464.213</td>
<td>180.5</td>
<td>0.0298</td>
<td>372.7</td>
<td></td>
</tr>
<tr>
<td>209</td>
<td>2,2',3,3',4,4',5,5',6,6'</td>
<td>2051-24-3</td>
<td>498.658</td>
<td>309</td>
<td>0.00164</td>
<td>393.6</td>
<td></td>
</tr>
</tbody>
</table>

* Assuming ∆S<sub> fus </sub> = 56 J/mol K.
### TABLE 7.2.2
Summary of selected physical-chemical properties of some PCB congeners at 25 °C

<table>
<thead>
<tr>
<th>IUPAC no.</th>
<th>Congener</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry's law const. H/(Pa·m²/mol) calculated P/C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>P/Pa</td>
<td>P_P/Pa</td>
<td>S/(g/m³)</td>
</tr>
<tr>
<td>0</td>
<td>Biphenyl</td>
<td>1.3</td>
<td>3.50</td>
<td>7</td>
</tr>
<tr>
<td>1</td>
<td>2-</td>
<td>2.04</td>
<td>2.5</td>
<td>5.5</td>
</tr>
<tr>
<td>2</td>
<td>3-</td>
<td>1</td>
<td>1</td>
<td>2.5</td>
</tr>
<tr>
<td>3</td>
<td>4-</td>
<td>0.271</td>
<td>0.91</td>
<td>1.2</td>
</tr>
<tr>
<td>4</td>
<td>2,2'-</td>
<td>0.265</td>
<td>0.59</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>2,4-</td>
<td>0.254</td>
<td>0.254</td>
<td>1.25</td>
</tr>
<tr>
<td>8</td>
<td>2,4'</td>
<td>0.18</td>
<td>0.18</td>
<td>2</td>
</tr>
<tr>
<td>9</td>
<td>2,5-</td>
<td>0.027</td>
<td>0.030</td>
<td>0.354</td>
</tr>
<tr>
<td>10</td>
<td>2,6-</td>
<td>0.008</td>
<td>0.0358</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>3,3'</td>
<td>0.105</td>
<td>0.120</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>3,4-</td>
<td>0.0048</td>
<td>0.080</td>
<td>0.06</td>
</tr>
<tr>
<td>14</td>
<td>3,5-</td>
<td>0.143</td>
<td>0.220</td>
<td>0.4</td>
</tr>
<tr>
<td>15</td>
<td>4,4'-</td>
<td>0.132</td>
<td>0.441</td>
<td>0.14</td>
</tr>
<tr>
<td>18</td>
<td>2,2',5-</td>
<td>0.0384</td>
<td>0.090</td>
<td>0.2</td>
</tr>
<tr>
<td>26</td>
<td>2,3',5-</td>
<td>0.0136</td>
<td>0.003</td>
<td>0.08</td>
</tr>
<tr>
<td>28</td>
<td>2,4',4'</td>
<td>0.0008</td>
<td>0.0582</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>2,4-</td>
<td>0.00225</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>2,3',4'-</td>
<td>0.0054</td>
<td>0.02</td>
<td>0.09</td>
</tr>
<tr>
<td>33</td>
<td>3,4',4'-</td>
<td>0.0016</td>
<td>0.0548</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>3,4',5'-</td>
<td>0.0049</td>
<td>0.02</td>
<td>0.03</td>
</tr>
<tr>
<td>40</td>
<td>2,2',3,3v-</td>
<td>0.00025</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>2,2',3,5-</td>
<td>0.0054</td>
<td>0.02</td>
<td>0.09</td>
</tr>
<tr>
<td>47</td>
<td>2,2',4,4'</td>
<td>0.0016</td>
<td>0.0548</td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>2,2',4,5'</td>
<td>0.0049</td>
<td>0.02</td>
<td>0.03</td>
</tr>
<tr>
<td>52</td>
<td>2,2',5,5'</td>
<td>0.00225</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>2,2',5,6'</td>
<td>0.00025</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>2,2',6,6'</td>
<td>0.0054</td>
<td>0.02</td>
<td>0.09</td>
</tr>
<tr>
<td>60</td>
<td>2,3,4,4'</td>
<td>0.0016</td>
<td>0.0548</td>
<td></td>
</tr>
<tr>
<td>61</td>
<td>2,3,4,5-</td>
<td>0.00025</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>2,3,5,6-</td>
<td>0.0054</td>
<td>0.02</td>
<td>0.09</td>
</tr>
<tr>
<td>66</td>
<td>2,3',4,4'</td>
<td>0.00225</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>Compound</td>
<td>m/z</td>
<td>pCBB</td>
<td>logKow</td>
<td>logKoc</td>
</tr>
<tr>
<td>----------</td>
<td>-----</td>
<td>------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>2,4,4',6-</td>
<td>75</td>
<td>2.091</td>
<td>0.312</td>
<td>6.21</td>
</tr>
<tr>
<td>3,3',4,4'</td>
<td>77</td>
<td>0.002</td>
<td>0.001</td>
<td>6.5</td>
</tr>
<tr>
<td>3,3',5,5'</td>
<td>80</td>
<td>0.0012</td>
<td>0.0004</td>
<td>0.949</td>
</tr>
<tr>
<td>2,2',3,4,5-</td>
<td>86</td>
<td>0.00927</td>
<td>0.0504</td>
<td>0.02</td>
</tr>
<tr>
<td>2,2',3,4,5'-</td>
<td>87</td>
<td>0.00304</td>
<td>0.00227</td>
<td>0.004</td>
</tr>
<tr>
<td>2,2',3,4,6-</td>
<td>88</td>
<td>0.012</td>
<td>0.0368</td>
<td>0.200</td>
</tr>
<tr>
<td>2,2',4,5,5'-</td>
<td>101</td>
<td>0.00109</td>
<td>0.00364</td>
<td>0.01</td>
</tr>
<tr>
<td>2,2',4,6,6'-</td>
<td>104</td>
<td>0.00434</td>
<td>0.0156</td>
<td>0.0478</td>
</tr>
<tr>
<td>2,3,3',4,4'</td>
<td>105</td>
<td>0.00012</td>
<td>0.0041</td>
<td>0.0012</td>
</tr>
<tr>
<td>2,3,3',4,6-</td>
<td>110</td>
<td>0.004</td>
<td>0.0123</td>
<td>6.3</td>
</tr>
<tr>
<td>2,3,4,5,6-</td>
<td>116</td>
<td>0.008</td>
<td>0.0245</td>
<td>0.227</td>
</tr>
<tr>
<td>2,2',3,3',4,4'-</td>
<td>128</td>
<td>1.98 × 10^{-5}</td>
<td>0.00034</td>
<td>0.0006</td>
</tr>
<tr>
<td>2,2',3,3',4,5-</td>
<td>129</td>
<td>0.0006</td>
<td>0.00166</td>
<td>0.0064</td>
</tr>
<tr>
<td>2,2',3,3',5,5-</td>
<td>134</td>
<td>0.00004</td>
<td>0.00111</td>
<td>0.0060</td>
</tr>
<tr>
<td>2,2',3,3',6,6'-</td>
<td>136</td>
<td>0.0008</td>
<td>0.00222</td>
<td>0.0167</td>
</tr>
<tr>
<td>2,2',4,4',5,5'-</td>
<td>153</td>
<td>0.000119</td>
<td>0.00007</td>
<td>0.001</td>
</tr>
<tr>
<td>2,2',4,4',6,6'-</td>
<td>155</td>
<td>0.00048</td>
<td>0.00345</td>
<td>0.002</td>
</tr>
<tr>
<td>2,2',4,4',6,6'-</td>
<td>171</td>
<td>2.73 × 10^{-5}</td>
<td>0.00022</td>
<td>0.002</td>
</tr>
<tr>
<td>2,2',4,5,5',6-</td>
<td>185</td>
<td>0.00045</td>
<td>0.00114</td>
<td>0.0188</td>
</tr>
<tr>
<td>2,2',4,5,6,6'-</td>
<td>194</td>
<td>0.0002</td>
<td>0.00047</td>
<td>0.00962</td>
</tr>
<tr>
<td>2,2',3,3',4,4',5,5'-</td>
<td>202</td>
<td>2.66 × 10^{-5}</td>
<td>0.0006</td>
<td>0.0003</td>
</tr>
<tr>
<td>2,2',3,3',4,4',5,5',6-</td>
<td>206</td>
<td>1.96 × 10^{-7}</td>
<td>1.17 × 10^{-5}</td>
<td>0.00011</td>
</tr>
<tr>
<td>2,2',3,3',4,4',5,5',6,6'-</td>
<td>207</td>
<td>0.0002</td>
<td>0.00047</td>
<td>0.00962</td>
</tr>
<tr>
<td>2,2',3,3',4,5,5',6,6'-</td>
<td>208</td>
<td>1.8 × 10^{-5}</td>
<td>3.88 × 10^{-5}</td>
<td>0.00130</td>
</tr>
<tr>
<td>2,2',3,3',4,5,5',6,6'-</td>
<td>209</td>
<td>5.02 × 10^{-8}</td>
<td>3.06 × 10^{-8}</td>
<td>1.0 × 10^{-6}</td>
</tr>
<tr>
<td>2,2',3,3',4,5,5',6,6'-</td>
<td>210</td>
<td>5.02 × 10^{-7}</td>
<td>3.06 × 10^{-7}</td>
<td>1.0 × 10^{-6}</td>
</tr>
<tr>
<td>2,2',3,3',4,5,5',6,6'-</td>
<td>211</td>
<td>5.02 × 10^{-8}</td>
<td>3.06 × 10^{-8}</td>
<td>1.0 × 10^{-6}</td>
</tr>
</tbody>
</table>
## TABLE 7.2.3
Summary of physical properties of PCB isomer groups and Aroclor mixtures

<table>
<thead>
<tr>
<th>PCB isomer group</th>
<th>CAS no.</th>
<th>Molecular weight, MW g/mol</th>
<th>Cl no.</th>
<th>m.p. °C</th>
<th>Fugacity ratio, F range at 25°C</th>
<th>Le Bas molar volume, V_M (cm³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biphenyl</td>
<td>92-52-4</td>
<td>154.2</td>
<td>0</td>
<td>71</td>
<td>0.352</td>
<td>184.6</td>
</tr>
<tr>
<td>Monochloro-</td>
<td>27323-18-8</td>
<td>188.7</td>
<td>1</td>
<td>25.1–78</td>
<td>0.299–1.0</td>
<td>205.5</td>
</tr>
<tr>
<td>Dichloro-</td>
<td>25512-42-9</td>
<td>223.1</td>
<td>2</td>
<td>24.4–149</td>
<td>0.0594–1.0</td>
<td>226.4</td>
</tr>
<tr>
<td>Trichloro-</td>
<td>25323-68-6</td>
<td>257.5</td>
<td>3</td>
<td>28.1–102</td>
<td>0.173–0.932</td>
<td>247.3</td>
</tr>
<tr>
<td>Tetrachloro-</td>
<td>26914-33-0</td>
<td>292.0</td>
<td>4</td>
<td>47–164</td>
<td>0.042–0.606</td>
<td>268.2</td>
</tr>
<tr>
<td>Pentachloro-</td>
<td>25429-29-2</td>
<td>326.4</td>
<td>5</td>
<td>76.5–123</td>
<td>0.107–0.310</td>
<td>289.1</td>
</tr>
<tr>
<td>Hexachloro-</td>
<td>26601-64-9</td>
<td>360.9</td>
<td>6</td>
<td>70–201</td>
<td>0.0182–0.359</td>
<td>310</td>
</tr>
<tr>
<td>Heptachloro-</td>
<td>28655-71-2</td>
<td>395.3</td>
<td>7</td>
<td>109–162</td>
<td>0.0596–0.148</td>
<td>330.9</td>
</tr>
<tr>
<td>Octachloro-</td>
<td>31472-83-0</td>
<td>429.8</td>
<td>8</td>
<td>132–161</td>
<td>0.0452–0.0874474</td>
<td>351.8</td>
</tr>
<tr>
<td>Nonachloro-</td>
<td>53742-07-7</td>
<td>464.2</td>
<td>9</td>
<td>205–206</td>
<td>0.0163–0.0276</td>
<td>372.7</td>
</tr>
<tr>
<td>Decachloro-</td>
<td>2051-24-3</td>
<td>498.7</td>
<td>10</td>
<td>305</td>
<td>0.00167</td>
<td>393.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aroclor mixture</th>
<th>CAS no.</th>
<th>Molecular weight, MW g/mol</th>
<th>% Cl</th>
<th>No. of Cl/molecule</th>
<th>Fugacity ratio, F at 25°C</th>
<th>Density g/cm³ at 25°C</th>
<th>Distillation range °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aroclor 1016</td>
<td>12674-11-2</td>
<td>257</td>
<td>41</td>
<td>3</td>
<td>1.0</td>
<td>1.33</td>
<td>323–356</td>
</tr>
<tr>
<td>Aroclor 1221</td>
<td>111-042-82</td>
<td>192</td>
<td>20.5–21.5</td>
<td>1.15</td>
<td>1.0</td>
<td>1.15</td>
<td>275–320</td>
</tr>
<tr>
<td>Aroclor 1232</td>
<td>111-411-65</td>
<td>221</td>
<td>31.4–32.5</td>
<td>2.04</td>
<td>1.0</td>
<td>1.24</td>
<td>290–325</td>
</tr>
<tr>
<td>Aroclor 1242</td>
<td>534-692-19</td>
<td>261</td>
<td>42</td>
<td>3.1</td>
<td>1.0</td>
<td>1.35</td>
<td>325–366</td>
</tr>
<tr>
<td>Aroclor 1248</td>
<td>126-722-96</td>
<td>288</td>
<td>48</td>
<td>3.9</td>
<td>1.0</td>
<td>1.41</td>
<td>340–375</td>
</tr>
<tr>
<td>Aroclor 1254</td>
<td>110-976-91</td>
<td>327</td>
<td>54</td>
<td>4.96</td>
<td>1.0</td>
<td>1.5</td>
<td>365–390</td>
</tr>
<tr>
<td>Aroclor 1260</td>
<td>110-968-25</td>
<td>372</td>
<td>60</td>
<td>6.3</td>
<td>1.0</td>
<td>1.58</td>
<td>385–420</td>
</tr>
</tbody>
</table>
### TABLE 7.2.4
Summary of selected physical-chemical properties of PCB isomer groups and Aroclor mixtures at 20–25°C

<table>
<thead>
<tr>
<th>PCB isomer group</th>
<th>Aqueous solubility range</th>
<th>Vapor pressure range</th>
<th>Henry's law const.</th>
<th>log K_{OW} range</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S/(g/m³)</td>
<td>C_v/(mmol/m³)</td>
<td>C_l/(mmol/m³)</td>
<td>P_v/Pa</td>
</tr>
<tr>
<td>Biphenyl</td>
<td>7.0</td>
<td>45.39</td>
<td>129.7</td>
<td>1.30</td>
</tr>
<tr>
<td>Monochloro-</td>
<td>1.21–5.50</td>
<td>6.36-29.15</td>
<td>1.13-35.66</td>
<td>0.271-2.04</td>
</tr>
<tr>
<td>Dichloro-</td>
<td>0.060–2.0</td>
<td>0.269-8.96</td>
<td>4.56-10.14</td>
<td>0.0048-0.279</td>
</tr>
<tr>
<td>Trichloro-</td>
<td>0.015–0.40</td>
<td>0.0582-1.55</td>
<td>0.24-2.39</td>
<td>0.0136-0.143</td>
</tr>
<tr>
<td>Tetrachloro-</td>
<td>0.0043–0.010</td>
<td>0.0147-0.342</td>
<td>0.133-1.30</td>
<td>0.000059-0.0054</td>
</tr>
<tr>
<td>Pentachloro-</td>
<td>0.004–0.020</td>
<td>0.0123-0.0613</td>
<td>0.093-0.337</td>
<td>0.000304-0.0093</td>
</tr>
<tr>
<td>Hexachloro-</td>
<td>0.0004–0.0007</td>
<td>0.0011-0.002</td>
<td>0.0061-0.0286</td>
<td>0.000020-0.00159</td>
</tr>
<tr>
<td>Heptachloro-</td>
<td>0.000045–0.0002</td>
<td>0.00114-0.0051</td>
<td>0.0191-0.046</td>
<td>0.0000273</td>
</tr>
<tr>
<td>Octachloro-</td>
<td>0.0002–0.0003</td>
<td>0.00047-0.0007</td>
<td>0.0098-0.0158</td>
<td>0.0000266</td>
</tr>
<tr>
<td>Nonachloro-</td>
<td>0.00018–0.0012</td>
<td>0.000038-0.00024</td>
<td>0.00141-0.0146</td>
<td>-</td>
</tr>
<tr>
<td>Decachloro-</td>
<td>0.000761</td>
<td>0.0000024</td>
<td>0.0144</td>
<td>0.00000005</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aroclor mixture</th>
<th>Aqueous solubility range</th>
<th>Vapor pressure range</th>
<th>Henry's law const.</th>
<th>log K_{OW} range</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S/(g/m³)</td>
<td>C_v/(mmol/m³)</td>
<td>C_l/(mmol/m³)</td>
<td>P_v/Pa</td>
</tr>
<tr>
<td>Aroclor 1016</td>
<td>0.22-0.84</td>
<td>0.856-0.216</td>
<td>0.06-0.2</td>
<td>70-900</td>
</tr>
<tr>
<td>Aroclor 1221</td>
<td>0.59-5.0</td>
<td>0.307-26.0</td>
<td>0.89-2.0</td>
<td>34-450</td>
</tr>
<tr>
<td>Aroclor 1232</td>
<td>1.45</td>
<td>6.56-2.0</td>
<td>0.54</td>
<td>82-270</td>
</tr>
<tr>
<td>Aroclor 1242</td>
<td>0.1-0.75</td>
<td>0.383-2.87</td>
<td>0.05-0.13</td>
<td>45-130</td>
</tr>
<tr>
<td>Aroclor 1248</td>
<td>0.1-0.5</td>
<td>0.347-1.74</td>
<td>0.0085-0.11</td>
<td>5-300</td>
</tr>
<tr>
<td>Aroclor 1254</td>
<td>0.01-0.30</td>
<td>0.306-0.92</td>
<td>0.008-0.02</td>
<td>20-260</td>
</tr>
<tr>
<td>Aroclor 1260</td>
<td>0.003-0.08</td>
<td>0.00806-0.215</td>
<td>0.0002-0.012</td>
<td>20-60</td>
</tr>
</tbody>
</table>

* See discussion by Linkov et al. 2005.
### TABLE 7.2.5
Suggested half-life classes of polychlorinated biphenyls (PCBs) in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biphenyl</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Monochloro-</td>
<td>4</td>
<td>7</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Dichloro-</td>
<td>4</td>
<td>7</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Trichloro-</td>
<td>5</td>
<td>8</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Tetrachloro-</td>
<td>6</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Pentachloro-</td>
<td>6</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Hexachloro-</td>
<td>7</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Heptachloro-</td>
<td>7</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Octachloro-</td>
<td>8</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Nonachloro-</td>
<td>8</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Decachloro-</td>
<td>9</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

where,

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>~5</td>
<td>&lt; 10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~ 1 day)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~ 2 days)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5500 (~ 8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17000 (~ 2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55000 (~ 6 years)</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>

**FIGURE 7.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.
FIGURE 7.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

FIGURE 7.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated biphenyls.
FIGURE 7.2.4 Henry’s law constant versus Le Bas molar volume for polychlorinated biphenyls.

FIGURE 7.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated biphenyls.
7.3 REFERENCES


Bradley, R.S., Cleasby, T.G. (1953) The solubility of aromatic hydrocarbons in water.


Polychlorinated Biphenyls (PCBs)

© 2006 by Taylor & Francis Group, LLC


Cunningham, G.B. (1930) *Power* 72, 374. — reference from Boublík et al. 1984


Polychlorinated Biphenyls (PCBs)


Polychlorinated Biphenyls (PCBs)


Nirmalakhandan, N.N., Speece, R.E. (1989) Prediction of aqueous solubility of organic chemicals based on molecular structure. 2. Application to FNs, PCBs, PCDDs, etc. Environ. Sci. Technol. 23(6), 708–713.


Polychlorinated Biphenyls (PCBs)


Polychlorinated Biphenyls (PCBs)


8 Chlorinated Dibenzo-\( p \)-dioxins

CONTENTS

8.1 List of Chemicals and Data Compilations ................................................................. 2064
  8.1.1 Dibenzo-\( p \)-dioxin and chlorinated dibenzo-\( p \)-dioxins .................................... 2064
    8.1.1.1 Dibenzo-\( p \)-dioxin ....................................................................................... 2064
    8.1.1.2 1-Chlorodibenzo-\( p \)-dioxin . ....................................................................... 2067
    8.1.1.3 2-Chlorodibenzo-\( p \)-dioxin ....................................................................... 2070
    8.1.1.4 2,3-Dichlorodibenzo-\( p \)-dioxin ................................................................. 2073
    8.1.1.5 2,7-Dichlorodibenzo-\( p \)-dioxin ................................................................. 2076
    8.1.1.6 2,8-Dichlorodibenzo-\( p \)-dioxin ................................................................. 2080
    8.1.1.7 1,2,4-Trichlorodibenzo-\( p \)-dioxin ............................................................... 2083
    8.1.1.8 1,3,7-Trichlorodibenzo-\( p \)-dioxin ............................................................... 2086
    8.1.1.9 2,3,7-Trichlorodibenzo-\( p \)-dioxin ............................................................... 2089
    8.1.1.10 1,2,3,4-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2100
    8.1.1.11 1,2,3,7-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2102
    8.1.1.12 1,2,7,8-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2107
    8.1.1.13 1,3,7,8-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2109
    8.1.1.14 1,3,7,9-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2111
    8.1.1.15 2,3,7,8-Tetrachlorodibenzo-\( p \)-dioxin .................................................... 2119
    8.1.1.16 1,2,3,4,7-Pentachlorodibenzo-\( p \)-dioxin .............................................. 2123
    8.1.1.17 1,2,3,7,8-Pentachlorodibenzo-\( p \)-dioxin .............................................. 2126
    8.1.1.18 1,2,4,7,8-Pentachlorodibenzo-\( p \)-dioxin .............................................. 2128
    8.1.1.19 1,2,3,4,6,7,9-Heptachlorodibenzo-\( p \)-dioxin ...................................... 2133
    8.1.1.20 1,2,3,4,7,8-Hexachlorodibenzo-\( p \)-dioxin ........................................... 2136
    8.1.1.21 1,2,3,6,7,8-Hexachlorodibenzo-\( p \)-dioxin ........................................... 2139
    8.1.1.22 1,2,3,7,8,9-Hexachlorodibenzo-\( p \)-dioxin ........................................... 2141
    8.1.1.23 1,2,3,4,6,7,9-Hexachlorodibenzo-\( p \)-dioxin ...................................... 2146
    8.1.1.24 1,2,3,4,6,7,8-Heptachlorodibenzo-\( p \)-dioxin ...................................... 2148
    8.1.1.25 1,2,3,4,7,8,9-Heptachlorodibenzo-\( p \)-dioxin ...................................... 2154
    8.1.1.26 Octachlorodibenzo-\( p \)-dioxin .............................................................. 2159

8.2 Summary Tables and QSAR Plots ................................................................................. 2154
8.3 References ..................................................................................................................... 2159
8.1 LIST OF CHEMICALS AND DATA COMPILATIONS

8.1.1 DIBENZO-P-DIOXIN AND CHLORINATED DIBENZO-P-DIOXINS

8.1.1.1 Dibenzo-p-dioxin

Common Name: Dibenzo-p-dioxin
Synonym: dibenzo-1,4-dioxin
Chemical Name: dibenzo-p-dioxin
CAS Registry No: 262–12–4
Molecular Formula: C6H4O2C6H4
Molecular Weight: 184.191
Melting Point (°C):
120.5 (Lide 2003)
Boiling Point (°C):
266.0 (Rordorf 1986)
Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
143.82, 142.06 (calculated-liquid density, crystalline volume, Govers et al. 1990)
146.96 (liquid molar volume, Govers et al. 1995)
177.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHv (kJ/mol):
68.4 (Rordorf 1987)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
92.250 (Rordorf 1987)
93.6 (Li et al. 2004)
Enthalpy of Fusion, ΔHfus (kJ/mol):
23.2, 22.6 (obs., predicted, Rordorf 1986)
22.6 (Ruelle & Kesselring 1997)
23.2, 22.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
58.63, 57.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.116 (mp at 120.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.842*, 0.90 (generator column-HPLC/UV, generator column-GC/ECD; Shiu et al. 1988)
0.90* (generator column-GC/ECD, measured range 4–25°C, Doucette & Andren 1988a)
0.90* (generator column-GC, measured range 4–40°C, Doucette & Andren 1988a)
S/(mol/L) = 8.85 × 10⁻⁷ exp(0.067·t°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a)
log x = −2541/(T/K) − 1.476; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
ln x = 4.1680 – 6087.88/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
7.16 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.050 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
0.512; 0.251 (supercooled liquid P, quoted exptl., calculated-SOFA Solubility-parameter-based-model, Govers & Krop 1998)
log (P/Pa) = 14.91018 – 4820.43/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
Chlorinated Dibenzo-\(p\)-dioxins

0.389; 0.251 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
0.107* (30°C, Knudsen effusion method, measured range 30–60°C Li et al. 2002)

\[
\ln \left( \frac{P}{Pa} \right) = \frac{(34.944 \pm 0.444) - (11259 \pm 141)}{(T/K)}; \text{ temp range 303–333 K} \] (Knudsen effusion technique, Li et al. 2002, 2004)
\[
\ln \left( \frac{P}{Pa} \right) = 34.319 - \frac{11095}{(T/K)}; \text{ temp range 298–398 K} \] (regression eq. of Rordorf 1989 data, Li et al. 2004)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):
12.40 (calculated-P/C, Shiu et al. 1987; 1988)
10.96 (calculated-SOFA model, Govers & Krop 1998)
15.85; 10.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log \(K_{OW}\):
4.31, 4.48, 4.38; 4.38, 4.46, 4.52 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
4.26, 4.65 (Doucette 1985)
4.17, 4.46 (HPLC-RT correlation, Sarna et al. 1984)
4.26, 4.01; 4.34, 4.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
4.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)
4.37 (generator column-GC, Doucette & Andren 1987)
4.18 (HPLC-RT correlation, Doucette & Andren 1988b)
4.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{OA}\) at 25°C:

Bioconcentration Factor, log BCF:
4.49; 4.68 (lipid based BCF, guppy, quoted expvl., calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

Sorption Partition Coefficient, log \(K_{OC}\):
4.01 (derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
Volatilization:
\[
\text{Volatilization:} \] (for reaction with OH radical, k\(_{OH}\) with NO\(_3\) radical and k\(_{O3}\) with O\(_3\) as indicated *data at other temperatures see reference:
\[
k_{OH} = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ corresponding to an atmospheric lifetime } \tau \approx 7 \text{ h at room temp. (Atkinson 1987a)}
\]
\[
k_{OH}(\text{calc}) = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1987b)}
\]
\[
k_{OH} = 37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{, calculated tropospheric lifetime } \tau = 0.4 \text{ d based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule cm}^{-3} \text{ (Atkinson 1991)}
\]
\[
k_{OH} = 1.48 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and the calculated tropospheric lifetime } \tau = 1.0 \text{ d, } k_{NO3} = 3.9 \times 10^{-27} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated lifetime } \tau = 4.9 \text{ d, and } k_{O3} < 5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime } \tau > 330 \text{ d at } 297 \pm 2 \text{ K (Kwok et al. 1994)}
\]
\[
k_{OH}(\text{exptl}) = 14.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ corresponding to a tropospheric lifetime of } 1.0 \text{ d (Kwok et al. 1995)}
\]
\[
k_{OH}^{*} = 12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 345–385 \text{ K; and } k_{OH}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated atmospheric lifetime } \tau = 24 \text{ h based on gas-phase OH reactions (Brubaker & Hites 1998)}
\]

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k\(_1\)) and Elimination (k\(_2\)) Rate Constants:
Half-Lives in the Environment:

Air: room temp. gas-phase reaction rate constant $k = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical corresponding to an atmospheric lifetime of about 7 h (Atkinson 1987a);
tropospheric lifetime $\tau = 0.4 \text{ d}$ calculated for dibenzo-$p$-dioxin based on the gas-phase reaction with OH radical (Atkinson 1991);
tropospheric lifetimes: $\tau(\text{calc}) = 1.0 \text{ d}, 4.9 \text{ d}$ and >330 d for reactions with OH radical, NO$_3$ radical and O$_3$, respectively at room temp. (Kwok et al. 1994);
tropospheric lifetime $\tau(\text{calc}) = 1.0 \text{ d}$ with respect to reaction with the OH radical (Kwok et al. 1995).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:

### TABLE 8.1.1.1.1
Reported aqueous solubilities and vapor pressures of dibenzo-$p$-dioxin at various temperatures and the reported temperature dependence equations

<table>
<thead>
<tr>
<th>T/°C</th>
<th>S/g·m$^{-3}$</th>
<th>T/°C</th>
<th>S/g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.205</td>
<td>25</td>
<td>0.055</td>
</tr>
<tr>
<td>15</td>
<td>0.460</td>
<td>50</td>
<td>0.98</td>
</tr>
<tr>
<td>25</td>
<td>0.842</td>
<td>75</td>
<td>12.0</td>
</tr>
<tr>
<td>35</td>
<td>1.762</td>
<td>100</td>
<td>97</td>
</tr>
<tr>
<td>45</td>
<td>3.262</td>
<td>125</td>
<td>630</td>
</tr>
</tbody>
</table>

$\Delta H_{\text{sub}}/\text{(kJ mol}^{-1}\text{)} = 50.68$
for 5–45 °C

$S/(\text{mol/L}) = a \cdot \exp[b(t/°C)]$

$a = 8.85 \times 10^{-7}$

$b = 0.067$

OR:

$\ln x = A - B/(T/K)$

$A = -1.476$

$B = 2541$

### FIGURE 8.1.1.1.1
Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for dibenzo-$p$-dioxin.
8.1.1.2 1-Chlorodibenzo-\(\mu\)-dioxin

![Chemical Structure](image)

Common Name: 1-Chlorodibenzo-\(\mu\)-dioxin  
Synonym: 1-CDD, 1-MCDD  
Chemical Name: 1-chlorodibenzo-\(\mu\)-dioxin  
CAS Registry No: 39227–53–7  
Molecular Formula: \(\text{C}_6\text{H}_4\text{O}_2\text{C}_6\text{H}_3\text{Cl}\)  
Molecular Weight: 218.636

Melting Point (°C):  

Boiling Point (°C):  
296.0 (Rordorf 1986)

Density (g/cm\(^3\) at 20°C):  
Molar Volume (cm\(^3\)/mol):
- 157.41, 158.07 (calculated-liquid density, crystalline volume, Govers et al. 1990)
- 156.19 (liquid molar volume, Govers et al. 1995)
- 197.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
- 76.2 (Rordorf 1987)

Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
- 98.55 (Rordorf 1987)
- 100.5 (Li et al. 2004)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
- 23.2, 22.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
- 56.0 (Rordorf 1986, 1987, 1989)
- 61.34, 58.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), \(F\): 0.164 (mp at 105.5°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.417* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

\[\ln x = -0.68385 - 4912.15/(T/K)\]; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
- 1.51 (supercooled liquid \(S_L\), GC-RI correlation; Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

\[\log (P/Pa) = 15.35327 - 5150.4/(T/K)\]; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.0275 (supercooled liquid \(P_L\), GC-RI correlation, Wang & Wong 2002)

\[\ln (P/Pa) = 35.353 - 11859/(T/K)\]; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

\[\ln (P/Pa) = (36.087 \pm 0.293) - (12085 \pm 96)/(T/K)\]; temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):
- 8.38 (calculated-P/C, Shiu et al. 1988)
- 6.31; 4.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
- 7.76; 5.75 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
Octanol/Water Partition Coefficient, $\log K_{OW}$:
- 4.97, 5.20, 5.25; 5.05, 5.18, 5.23 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 4.91, 5.18 (HPLC-RT correlation, Sarna et al. 1984)
- 4.81, 4.52; 4.91, 5.74 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 4.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 5.05 (recommended, Hansch et al. 1995)
- 4.99 (GC-RI correlation; Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
- 7.86*; 8.34 (generator column-GC; calculated, Harner et al. 2000)
- $\log K_{OA} = -2.88 + 3200/(T/K)$; temp range 10–40°C (Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:
- 5.17; 5.08 (lipid wt base, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:
- 5.46 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated *data at other temperatures see reference:
  - $k_{OH}(\text{calc}) = 32 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, calculated tropospheric lifetime $\tau = 0.5$ d based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ (Atkinson 1991)
  - $k_{OH}(\text{exptl}) = 4.7 \times 10^{-12}$ cm$^3$·molecule$^{-1}$·s$^{-1}$, $k_{OH}(\text{calc}) = 8.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$·s$^{-1}$, corresponding to a tropospheric lifetime of 1.0 d (relative rate method, Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: tropospheric lifetime $\tau = 0.5$ d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
  - calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
TABLE 8.1.1.2.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1-chlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Shiu et al. 1988</strong></td>
<td><strong>Rordorf 1987, 1989</strong></td>
<td><strong>Harner et al. 2000</strong></td>
</tr>
<tr>
<td>generator column-HPLC/UV</td>
<td>gas saturation-GC</td>
<td>generator column-GC/ECD</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g \cdot m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>0.205</td>
<td>25</td>
</tr>
<tr>
<td>15</td>
<td>0.460</td>
<td>50</td>
</tr>
<tr>
<td>25</td>
<td>0.842</td>
<td>75</td>
</tr>
<tr>
<td>35</td>
<td>1.762</td>
<td>100</td>
</tr>
<tr>
<td>45</td>
<td>3.262</td>
<td>125</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}/(kJ \cdot mol^{-1}) = 40.85$ for 5–45°C

$\Delta H_{v}/(kJ \cdot mol^{-1}) = 76.2$

$\Delta H_{subl}/(kJ \cdot mol^{-1}) = 98.55$

$\Delta H_{fus}/(kJ \cdot mol^{-1}) = 21.4$

$\Delta S_{fus}/(J \cdot mol^{-1} \cdot K^{-1}) = 56.0$

enthalpy of phase change

$\Delta H_{OA}/(kJ \cdot mol^{-1}) = 61.30$

FIGURE 8.1.1.2.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 1-chlorodibenzo-p-dioxin.
8.1.1.3 2-Chlorodibenzo-p-dioxin

Common Name: 2-Chlorodibenzo-p-dioxin
Synonym: 2-CDD, 2-MCDD
Chemical Name: 2-chlorodibenzo-p-dioxin
CAS Registry No: 39227–54–8
Molecular Formula: C₆H₄O₂C₆H₃Cl
Molecular Weight: 218.636
Melting Point (°C): 88–89 (Pohland & Yang 1972)
Boiling Point (°C): 298.0 (Rordorf 1986)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
154.85, 155.15 (calculated-liquid density, crystalline volume, Govers et al. 1990)
153.09 (liquid molar volume, Govers et al. 1995)
197.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
78.2 (Rordorf 1987)
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):
97.16 (Rordorf 1987)
98.1 (Li et al. 2004)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
23.1, 18.5 (obs., predicted, Rordorf 1986)
18.5 (Ruelle & Kesselring 1997)
23.1, 21.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
51 (Rordorf 1987, 1989)
63.78, 57.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.236 (mp at 89°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.278*, 0.319 (generator column-HPLC/UV, generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1988)
0.319* (generator column-GC/ECD, measured range 3.9–39°C, Doucette & Andren 1988a)
S/(mol/L) = 4.88 × 10⁻⁷ exp(0.048·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
log x = −1777/(T/K) − 1.566, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
ln x = 4.093418 − 6448/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
1.44 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.017* (gas saturation-GC, Rordorf 1985a,b,1986,1987,1989)
0.016 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
log (P/Pa) = 15.2463 − 5071.88/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0262 (GC-RI correlation, Wang & Wong 2002)
Chlorinated Dibenzo-\(\beta\)-dioxins

\[
\ln \left( \frac{P}{P_0} \right) = 35.106 - \frac{11679}{T/\text{K}}; \text{ temp range } 298-398 \text{ K (regression eq. of Rordorf 1989 data, Li et al. 2004)}
\]
\[
\ln \left( \frac{P}{P_0} \right) = (35.549 \pm 0.415) - \frac{(11794 \pm 134)}{T/\text{K}}, \text{ temp range } 308-343 \text{ K (Knudsen effusion technique, Li et al. 2004)}
\]

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):

- 14.82 (calculated-P/C, Shiu et al. 1988)
- 12.60; 4.57 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 7.586; 4.57 (GC-R/ correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):

- 5.36, 5.66, 5.71; 5.45, 5.64, 5.69 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 5.45, 5.64 (HPLC-RT correlation, Sarna et al. 1984)
- 5.33, 5.00; 5.45, 5.29 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 5.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 4.94 (generator column-GC/ECD, Doucette & Andren 1987)
- 4.98 (HPLC-RT correlation, Doucette & Andren 1988b)
- 5.45 (recommended, Hansch et al. 1995)
- 5.01 (GC-R/ correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, \(\log K_{\text{oa}}\):

Bioconcentration Factor, \(\log BCF\):

- 5.09 (guppy, Loonen et al. 1994)
- 5.09; 5.12 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, \(\log K_{\text{oc}}\):

- 3.92 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 5.35 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t\_\text{\(1/2\)}\):

Volatilization:

Photolysis: photodegradation \(t\_\text{\(1/2\)} = 10\) min with simulated sunlight in aerated aqueous suspension of semiconductor \(\text{TiO}_2\) at 4.0 g/L and \(\text{pH}\) 3 (Pelizzetti et al. 1988)

photodegradation \(k = 1.81\) h\(^{-1}\) with \(t\_\text{\(1/2\)} = 0.38\) h when loaded on \(\text{TiO}_2\) film under UV \((\lambda > 300 \text{ nm})\) or solar light irradiation in the air (Choi et al. 2000).

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO}_3}\) with \(\text{NO}_3\) radical and \(k_{\text{O}_3}\) with \(\text{O}_3\) or as indicated, *data at other temperatures see reference:

- \(k_{\text{OH}} = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\), calculated tropospheric lifetime \(\tau = 0.5\) d for a mono-chlorinated dioxin with a 12-h average daytime OH radical concn of \(1.5 \times 10^6\) molecule/cm\(^3\) (Atkinson 1991)
- \(k_{\text{OH(exptl)}} = 4.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\), \(k_{\text{OH(calc)}} = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a calculated tropospheric lifetime \(\tau = 3.0\) d at room temp. (relative rate method, Kwok et al. 1995)
- \(k_{\text{OH(calc)}} = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime \(\tau = 0.5\) d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime for mono-chlorinated dioxin was \(3.0\) d for the gas-phase reaction with OH radical (Kwok et al. 1995).

first-order photodegradation \(k = 1.81\) h\(^{-1}\) with \(t\_\text{\(1/2\)} = 0.38\) h when loaded on \(\text{TiO}_2\) film under UV \((\lambda > 300 \text{ nm})\) or solar light irradiation in the air (Choi et al. 2000).
Surface water: $t_{1/2} = 10$ min irradiated under simulated sunlight in aerated aqueous suspension of semiconductor TiO$_2$ at 4.0 g/L and pH 3 (Pelizzetti et al. 1988).

Groundwater:

Sediment:

Soil:

Biota:

### TABLE 8.1.1.3.1

Reported aqueous solubilities and vapor pressures of 2-chlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Temperature ($^\circ$C)</th>
<th>Aqueous solubility ($S$/g·m$^{-3}$)</th>
<th>Vapor pressure (P/Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.0603</td>
<td>0.017</td>
</tr>
<tr>
<td>15</td>
<td>0.137</td>
<td>0.36</td>
</tr>
<tr>
<td>25</td>
<td>0.278</td>
<td>4.80</td>
</tr>
<tr>
<td>35</td>
<td>0.653</td>
<td>45.0</td>
</tr>
<tr>
<td>45</td>
<td>1.109</td>
<td>320</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}$(kJ mol$^{-1}$) = 34.0

4–32 °C

$\Delta H_{sol}$(kJ mol$^{-1}$) = 53.35

5–45 °C

$\Delta H_{fus}$(kJ mol$^{-1}$) = 18.5

$\Delta S_{fus}$(J mol$^{-1}$ K$^{-1}$) = 51

$\Delta H_{sub}$(kJ mol$^{-1}$) = 97.16

$\Delta H_{vap}$(kJ mol$^{-1}$) = 78.1

**FIGURE 8.1.1.3.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2-chlorodibenzo-p-dioxin.
2,3-Dichlorodibenzo-p-dioxin

Common Name: 2,3-Dichlorodibenzo-p-dioxin
Synonym: 2,3-DCDD
Chemical Name: 2,3-dichlorodibenzo-p-dioxin
CAS Registry No: 29446–15–9
Molecular Formula: C₁₆H₄O₂C₆H₂Cl₂
Molecular Weight: 253.081
Melting Point (°C): 163–164 (Pohland & Yang 1972)
Density (g/cm³ at 20°C):
- 164.07 (calculated-liquid density, Govers et al. 1990)
- 162.67 (liquid molar volume, Govers et al. 1995)
- 218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
- 77.8 (Rordorf 1987)
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):
- 106.23 (Rordorf 1987)
- 106.2 (Li et al. 2004)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
- 26.7 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.0433 (mp at 164°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.0149* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)
  ln x = 0.07859 − 6173.64/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
- 0.297 (GC-RI correlation, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.00039* (gas saturation-GC, Rordorf 1985a, b, 1986, 1989)
- 0.0004 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- 0.0020 (GC-RI correlation, Wang & Wong 2002)
  log (P/μmHg) = 48.98 − 6446/(T/K) − 12.569·log (T/K) (supercooled liquid P_L, Kirchhoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
  ln (P/Pa) = 35.096 − 12804/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
  ln (P/Pa) = (35.081 ± 0.374) − (12771 ± 134)/(T/K); temp range 338–378 K (Knudsen effusion technique, Li et al. 2004)
Henry’s Law Constant (Pa m³/mol at 25°C):
- 6.61 (calculated-P/C, Shiu et al. 1988)
- 6.61; 2.51 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 3.80; 2.51 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 4.70 (calculated, Kaiser 1983)
- 6.23, 5.60 (calculated-QSAR, quoted, Fiedler & Schramm 1990)
- 5.77 (calculated-SOFA model, Govers & Krop 1998)
- 5.738 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.80; 5.77 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C:
- 8.50 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- 5.41 (lipid wt based, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{OC}$:
- 4.73 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 6.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
  - Photolysis:
    - Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{N\text{O}_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
      - $k_{OH}(\text{calc}) = 22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)
      - $k_{OH} = (22 - 28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5$–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
      - $k_{OH}(\text{calc}) = (5.9 - 7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0$–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)
      - $k_{OH}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

- Hydrolysis:
- Biodegradation:
- Biotransformation:

- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_2 = 0.092 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:
- Air: tropospheric lifetime $\tau = 0.5$–0.7 d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
  - calculated tropospheric lifetime $\tau = 2.0$–2.4 d for the reaction with OH radical (Kwok et al. 1995).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
  - Biot: mean biological $t_{1/2}$ ~2 d in rainbow trout (Niimi 1986);
    - biological $t_{1/2} = 7 \text{ d}$ in rainbow trout (Niimi & Oliver 1986);
    - biological $t_{1/2} = 2$–7 d in trout (Niimi 1987).
### TABLE 8.1.1.4.1
Reported aqueous solubilities and vapor pressures of 2,3-dichlorodibenzo-
\( p \)-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>generator column-HPLC/UV</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/g \cdot m^{-3} )</td>
</tr>
<tr>
<td>5</td>
<td>0.00368</td>
</tr>
<tr>
<td>15</td>
<td>0.00716</td>
</tr>
<tr>
<td>25</td>
<td>0.0149</td>
</tr>
<tr>
<td>35</td>
<td>0.0304</td>
</tr>
<tr>
<td>45</td>
<td>0.0586</td>
</tr>
</tbody>
</table>

\( \Delta H_{\text{sol}}/(kJ \cdot mol^{-1}) = 51.3 \)

5–45 °C

\( \Delta H_{\text{fus}}/(kJ \cdot mol^{-1}) = 26.7 \)

\( \Delta S_{\text{fus}}/(J \cdot mol^{-1} \cdot K^{-1}) = 61 \)

\( \Delta H_{\text{subl}}/(kJ \cdot mol^{-1}) = 106.23 \)

\( \Delta H_{V}/(kJ \cdot mol^{-1}) = 77.8 \)

\( \Delta H_{\text{fus}}/(kJ \cdot mol^{-1}) = 26.7 \)

\( \Delta S_{\text{fus}}/(J \cdot mol^{-1} \cdot K^{-1}) = 61 \)

FIGURE 8.1.1.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,3-dichlorodibenzo-
\( p \)-dioxin.
8.1.1.5 2,7-Dichlorodibenzo-p-dioxin

Common Name: 2,7-Dichlorodibenzo-p-dioxin
Synonym: 2,7-DCDD
Chemical Name: 2,7-dichlorodibenzo-p-dioxin
CAS Registry No: 33857–26–0
Molecular Formula: ClC₆H₃O₂C₆H₃Cl
Molecular Weight: 253.081
Melting Point (°C):
   210 (Lide 2003)
Boiling Point (°C):
   374.5 (calculated, Rordorf 1987, 1989)
Density (g/cm³):
   1.647 (calculated, Boer et al. 1972)
Molar Volume (cm³/mol):
   165.88, 162.89 (calculated-liquid density, crystalline volume, Govers et al. 1990)
   162.87 (liquid molar volume, Govers et al. 1995)
   218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
   76.4 (Rordorf 1987)
Enthalpy of Sublimation, $\Delta H_{sub}$ (kJ/mol):
   105.51 (Rordorf 1987)
   113.8 (Li et al. 2004)
Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
   26.8 (Rordorf 1986, 1987; Ruelle & Kesselring 1997)
Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{ fus} = 56$ J/mol K), F: 0.0188 (mp at 201°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00375* (generator column-HPLC/UV, Shiu et al. 1988)
0.00224 (generator column-GC/MS, Santl et al. 1994)
ln x = –3.48833 – 5543.9/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.311 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
log (P/Pa) = 14.60827 – 5523.34/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.00219 (GC-RI correlation, Wang & Wong 2002)
log (P/mmHg) = 49.61 – 6624/(T/K) – 12.569-log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
ln (P/Pa) = 33.637 – 12718/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (36.293 ± 0.648) – (13686 ± 245)/(T/K); temp range 358–393 K (Knudsen effusion technique, Li et al. 2004)
Chlorinated Dibenzo-p-dioxins

Henry’s Law Constant (Pa m³/mol at 25°C):

- 8.11 (calculated-P/C, Shiu et al. 1988)
- 6.98 (gas stripping-GC/MS, Santl et al. 1994)
- 8.13; 2.82 (quoted exp., calculated-SOFA model, Govers & Krop 1998)
- 3.89; 2.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

- 6.28, 6.64, 6.72; 6.38, 6.62, 6.71 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 6.62, 6.39 (HPLC-RT correlation, Sarna et al. 1984)
- 6.27, 5.86; 6.39, 6.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 5.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 6.38 (recommended, Sangster 1993)
- 6.38 (recommended, Hansch et al. 1995)
- 5.77 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equations.

- Additional data at other temperatures designated * are compiled at the end of this section:
  - log K_{oa} = –3.74 + 3610/(T/K); temp range 10–40°C (Harner et al. 2000)
  - 8.36*; 8.67 (generator column-GC; calculated, Harner et al. 2000)

Bioconcentration Factor, log BCF:

- 1.7, 2.9 (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.56, 3.68 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{oc}:

- 6.15 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:

Volatilization:

- Photolysis: photodegradation t_{½} = 46 min in an aqueous solution assisted by TiO₂ at 2.0 g/L under simulated sunlight (Barbeni et al. 1986)
- Photodegradation t_{½} = 1 h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO₂ at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)
- Photolysis k = 8.9 × 10⁻² min⁻¹ with t_{½} = 7.8 min in pure water, and rate constant k = 0.16 min⁻¹ with t_{½} = 4.3 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O’Keefe 2000).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

- k_{OH(calc)} = (26–28) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)
- k_{OH} = (22–28) × 10⁻¹² cm³ molecule⁻¹ s⁻¹, calculated tropospheric lifetime τ = 0.5–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5 × 10⁶ molecule/cm³ (Atkinson 1991)
- k_{OH(calc)} = (5.9–7.3) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a calculated tropospheric lifetime τ = 2.0–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)
- k_{OH(calc)} = 4.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Brubaker & Hites 1998)
- k_{OH} = 23 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K, measured temp range 355–395 K, and k_{OH(calc)} = 4.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, with a calculation lifetime τ = 65 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Biodegradation:

- Biotransformation: metabolic elimination k_{m} = 0.23 d⁻¹ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

Bioconcentration, Uptake (kₜ₁) and Elimination (kₜ₂) Rate Constants:

- k₂ = 0.462 d⁻¹ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
- kₜ₁ = 390 mL g⁻¹ d⁻¹; kₜ₂ = 0.23 d⁻¹ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)
- kₜ₁ = 543 d⁻¹; k₂ = 1.5 d⁻¹ (guppy, Gobas & Schrap 1990)
Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5–0.7 \text{ d}$ calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric calculated lifetime $\tau = 2.0–2.4 \text{ d}$ for the reaction with OH radical (Kwok et al. 1995);
calculated lifetime $\tau = 65 \text{ h}$ based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: photodegradation $t_{1/2} = 1 \text{ h}$ with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO$_2$ at 4.0 g/L and pH 3 (Pelizzetti et al. 1988);

photolysis rate constant $k = 8.9 \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 7.8 \text{ min}$ in pure water, and $k = 1.6 \times 10^{-1} \text{ min}^{-1}$ with $t_{1/2} = 4.3 \text{ min}$ in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O’Keefe 2000).

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 2 \text{ d}$ in rainbow trout (Niimi 1986);
biological $t_{1/2} = 2 \text{ d}$ in rainbow trout (Niimi & Oliver 1986);
biological $t_{1/2} = 2–7 \text{ d}$ in trout (Niimi 1987).

### TABLE 8.1.1.5.1

**Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,7-dichlorodibenzo- $p$-dioxin at various temperatures**

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-HPLC/UV</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>0.00109</td>
<td>25</td>
</tr>
<tr>
<td>15</td>
<td>0.00201</td>
<td>50</td>
</tr>
<tr>
<td>25</td>
<td>0.00375</td>
<td>75</td>
</tr>
<tr>
<td>35</td>
<td>0.00727</td>
<td>100</td>
</tr>
<tr>
<td>45</td>
<td>0.0134</td>
<td>125</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}$(kJ mol$^{-1}$) = 50.68

25 °C

Enthalpy of phase change

**$\Delta H_{OA}$**/(kJ mol$^{-1}$) = 69.0

**$\Delta H_{subl}$**/(kJ mol$^{-1}$) = 105.51

**$\Delta H_{fus}$**/(kJ mol$^{-1}$) = 26.8

**$\Delta S_{fus}$**/(J mol$^{-1}$ K$^{-1}$) = 55

$\log K_{OA} = a + b(T/K)$

a  -3.74

b  3610

© 2006 by Taylor & Francis Group, LLC
**FIGURE 8.1.1.5.1** Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 2,7-dichlorodibenzo-$p$-dioxin.
8.1.1.6 2,8-Dichlorodibenzo-p-dioxin

Common Name: 2,8-Dichlorodibenzo-p-dioxin
Synonym: 2,8-TCDD
Chemical Name: 2,8-dichlorodibenzo-p-dioxin
CAS Registry No: 38964–22–6
Molecular Formula: ClC₆H₃O₂C₆H₃Cl
Molecular Weight: 253.081
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
165.88, 167.2 (calculated-liquid density, crystalline volume, Govers et al. 1990)
160.63 (liquid molar volume, Govers et al. 1995)
218.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
84.1 (Rordorf 1987)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
109.01 (Rordorf 1987)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
23.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)
Entergy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), F: 0.058 (mp at 151°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0167* (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1988)
\ln x = –2.54177 – 5379/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.311 (supercooled liquid \( S_L \), GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
\log (P/Pa) = 15.25386 – 5699.96/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.00219 (supercooled liquid \( P_L \), GC-RI correlation, Wang & Wong 2002)
0.00150 (solid \( P_s \), gas saturation-GC/MS, Mader & Pankow 2003)
0.0260 (supercooled liquid \( P_L \), calculated from \( P_s \) assuming \( \Delta S_{fus} = 56 \) J/mol K, Mader & Pankow 2003)
\log (P_L/mmHg) = 49.89 – 6705/(T/K) – 12.569·\log (T/K) (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa m³/mol at 25°C):
2.13 (calculated-P/C, Shiu et al. 1988)
2.14; 2.29 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
3.89; 2.29 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 4.70 (calculated, Kaiser 1983)
- 5.60 (selected, Shiu et al. 1988)
- 5.68 (calculated-SOFA model, Govers & Krop 1998)
- 5.638 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.77; 5.68 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
- 5.34, 5.50, 5.75, 5.58 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.36*; 8.65 (generator column-GC; measured range 10–40°C; calculated, Harner et al. 2000)
- $\log K_{OA} = -3.74 + 3610/(T/K)$; temp range 10–40°C, (Harner et al. 2000)
- 8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:

- 2.77, 2.82 (goldfish: treated with metabolic inhibitor PBO, untreated, Sijm & Opperhuizen 1988)
- 5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{OC}$:


Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH}(calc) = (26–28) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (22–28) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, calculated tropospheric lifetime $\tau = 0.5–0.7$ d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^9$ molecule/cm$^3$ (Atkinson 1991)
- $k_{OH}(calc) = (5.9–7.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0–2.4$ d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation: metabolic elimination rate constant from goldfish was estimated to be 0.35 d$^{-1}$ (Sijm & Opperhuizen 1988).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 390$ L kg$^{-1}$d$^{-1}$; $k_2 = 0.23$ d$^{-1}$ (goldfish, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5 – 0.7$ d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.0 – 2.4$ d for the reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_\frac{1}{2} \sim 2$ d in rainbow trout (Niimi 1986); biological $t_\frac{1}{2} = 2–7$ d in trout (Niimi 1987).
TABLE 8.1.1.6.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,8-dichlorodibenzo-p-dioxon at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-HPLC/UV</td>
<td>gas saturation-GC</td>
<td>generator column-GC/ECD</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>5</td>
<td>0.00422</td>
<td>25</td>
</tr>
<tr>
<td>15</td>
<td>0.00859</td>
<td>50</td>
</tr>
<tr>
<td>25</td>
<td>0.0167</td>
<td>75</td>
</tr>
<tr>
<td>35</td>
<td>0.0275</td>
<td>100</td>
</tr>
<tr>
<td>45</td>
<td>0.0515</td>
<td>125</td>
</tr>
</tbody>
</table>

$\Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = 50.04$
$5-45 °C

$\Delta H_{\text{sub}}/(kJ \text{ mol}^{-1}) = 109.01$
$\Delta H_{\text{fus}}/(kJ \text{ mol}^{-1}) = 23.3$
$\Delta S_{\text{fus}}/(J \text{ mol}^{-1} \text{ K}^{-1}) = 55$

log $K_{OA} = a + b/(T/K)$
a = $-3.74$
b = $3610$

enthalpy of phase change
$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 69.0$

FIGURE 8.1.1.6.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 2,8-dichlorodibenzo-p-dioxin.
8.1.1.7 1,2,4-Trichlorodibenzo-\(p\)-dioxin

Common Name: 1,2,4-Trichlorodibenzo-\(p\)-dioxin
Synonym: 1,2,4-TCDD
Chemical Name: 1,2,4-trichlorodibenzo-\(p\)-dioxin
CAS Registry No: 39227–58–2
Molecular Formula: \(\text{C}_{12}\text{H}_5\text{Cl}_3\text{O}_2, \text{C}_6\text{H}_4\text{O}_2\text{C}_6\text{HCl}_3\)
Molecular Weight: 287.526

Boiling Point (\(^\circ\text{C}\)): 375.0 (calculated, Rordorf 1986, 1987, 1989)
Density (g/cm\(^3\) at 20\(^\circ\text{C}\)):
- 179.66 (calculated-liquid density, Govers et al. 1990)
- 173.60 (liquid molar volume, Govers et al. 1995)
- 239.7 (calculated-Le Bas method at normal boiling)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
- 83.9 (Rordorf 1987)

Enthalpy of Sublimation, \(\Delta H_{\text{subl}}\) (kJ/mol):
- 118.79 (Rordorf 1987)
- 121.0 (Li et al. 2004)

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
- 33.9 (Rordorf 1986, 1987)

Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):

Fugacity Ratio at 25\(^\circ\text{C}\) (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F: 0.0954 (mp at 129\(^\circ\text{C}\))

Water Solubility (g/m\(^3\) or mg/L at 25\(^\circ\text{C}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):
- 0.00841\* (generator column-HPLC/UV, measured range 5–45\(^\circ\text{C}\), Shiu et al. 1988)
- 0.00695 (generator column-GC/MS, Santl et al. 1994)

\[
\ln x = -2.4909 - 5626.95/(T/K); \text{temp range 5–50}^\circ\text{C} \text{ (regression eq. of literature data, Shiu & Ma 2000)}
\]

- 0.091 (supercooled liquid \(S_L\), GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25\(^\circ\text{C}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):
- 0.0001\* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)
- 0.0001 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

\[
\log (P/\text{Pa}) = 16.9148 - 6235.45/(T/K); \text{temp range 5–50}^\circ\text{C} \text{ (regression eq. from literature data, Shiu & Ma 2000)}
\]

- 0.000324 (supercooled liquid \(P_L\), GC-RI correlation, Wang & Wong 2002)

5.07 \times 10^{-4} (solid \(P_s\), gas saturation-GC/MS, Mader & Pankow 2003)

5.43 \times 10^{-3} (supercooled liquid \(P_L\), calculated from measured \(P_s\) assuming \(\Delta S_{\text{fus}} = 56\) J/mol K, Mader & Pankow 2003)

\[
\log (P_l/\text{mmHg}) = 47.18 - 6479/(T/K) - 12.028 \log (T/K) \text{ (supercooled liquid \(P_L\), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)}
\]
\[ \ln \left( \frac{P}{P_0} \right) = 38.948 - \frac{14358}{T/K} \]; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)  
\[ \ln \left( \frac{P}{P_0} \right) = 39.303 \pm 0.605 - \frac{14550 \pm 221}{T/K} \]; temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa·m³/mol at 25°C):
- 3.84  (calculated-P/C, Shiu et al. 1988)
- 3.64  (gas stripping-GC/MS, Santl et al. 1994)
- 3.72; 1.82  (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 2.29; 1.82  (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log \(K_{OW}\):
- 7.40, 7.77, 7.69; 7.47, 7.76, 7.68 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 7.45, 7.76 (HPLC-RT correlation, Sarna et al. 1984)
- 7.36, 6.86; 7.45, 7.11 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 6.45 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.47  (recommended, Hansch et al. 1995)
- 6.34  (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log \(K_{OA}\) at 25°C:
- 8.97  (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- 1.90, 3.10  (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.82, 3.95  (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.42  (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log \(K_{OC}\):
- 7.01  (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 5.87  (derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_\text{½}\):
- Volatilization: 
  - Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO\(_3\) radical and \(k_{O3}\) with O\(_3\) as or indicated, *data at other temperatures see reference: 
  - \(k\) (oxidative degradation rate of water dissolved PCDD by ozone) is \(1.27 \times 10^6\) L·g\(^{-1}\)·min\(^{-1}\) under alkaline conditions at pH 10 and 20°C (Paluschek & Scholz 1987)
  - \(k_{OH}(\text{calc}) = (21–22) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\)·s\(^{-1}\) at room temp. (Atkinson 1991)
  - \(k_{OH} = (17–22) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\)·s\(^{-1}\), calculated tropospheric lifetime \(\tau = 0.7–0.9\) d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of \(1.5 \times 10^6\) molecule/cm\(^3\) (Atkinson 1991)
  - \(k_{OH}(\text{calc}) = (4.5–5.9) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\)·s\(^{-1}\) with a calculated tropospheric lifetime \(\tau = 2.5–3.3\) d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)
- Biodegradation: 
- Biotransformation: 

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:
- \(k_1 = 601\) d\(^{-1}\); \(k_2 = 0.91\) d\(^{-1}\) (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:
- Air: tropospheric lifetime \(\tau = 0.7–0.9\) d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radical (Atkinson 1991); the calculated tropospheric lifetime \(\tau = 2.5–3.3\) d for the gas phase reaction with OH radical (Kwok et al. 1995).
- Surface water: oxidative degradation rate of water dissolved PCDD by ozone \(k = 1.27 \times 10^6\) L·g\(^{-1}\)·min\(^{-1}\) under alkaline conditions at pH 10 and 20°C (Paluschek & Scholz 1987).
Chlorinated Dibenzo-\(p\)-dioxins

Sediment:
Soil:
Biota: mean biological \( t_{1/2} \) ~ 10 d in rainbow trout (Niimi 1986);
\( t_{1/2} = 12 \text{ d} \) in rainbow trout (Niimi & Oliver 1986);
biological \( t_{1/2} = 12 \text{ d} \) in trout (Niimi 1987)

### TABLE 8.1.1.7.1
Reported aqueous solubilities and vapor pressures of 1,2,4-trichlorodibenzo-\(p\)-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>generator column-HPLC/UV</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m(^{-3})</td>
</tr>
<tr>
<td>5</td>
<td>0.00219</td>
</tr>
<tr>
<td>15</td>
<td>0.00477</td>
</tr>
<tr>
<td>25</td>
<td>0.00841</td>
</tr>
<tr>
<td>35</td>
<td>0.0167</td>
</tr>
<tr>
<td>45</td>
<td>0.0282</td>
</tr>
</tbody>
</table>

\( \Delta H_{vap}/(\text{kJ mol}^{-1}) = 83.9 \)

\( \Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 118.79 \)

\( \Delta H_{fus}/(\text{kJ mol}^{-1}) = 33.9 \)

\( \Delta S_{fus}/(\text{J mol}^{-1} \text{ K}^{-1}) = 84 \)

\( 5\text{–}45 \text{ °C} \)

**FIGURE 8.1.1.7.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4-trichlorodibenzo-\(p\)-dioxin.
8.1.1.8 1,3,7-Trichlorodibenzo-\(p\)-dioxin

Common Name: 1,3,7-Trichlorodibenzo-\(p\)-dioxin
Synonym: 1,3,7-TCDD
Chemical Name: 1,3,7-trichlorodibenzo-\(p\)-dioxin
CAS Registry No: 67026–17–5
Molecular Formula: \(\text{C}_{12}\text{H}_{5}\text{Cl}_{3}\text{O}_{2}\), \(\text{ClC}_{6}\text{H}_{3}\text{O}_{2}\text{C}_{6}\text{H}_{2}\text{Cl}_{2}\)
Molecular Weight: 287.526
Density (g/cm\(^3\) at 20°C): 170.18 (liquid molar volume, Govers et al. 1995)
239.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 86.4 (Rordorf 1987)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol): 116.2 (Rordorf 1987)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol): 28.4 (Rordorf 1986, 1987)
30.8, 25.7 (reported exptl., calculated, Chickos et al. 1999)
73.04, 61.0 (reported exptl., calculated, Chickos 1999)
Fugacity Ratio at 25°C (assuming \(\Delta S = 56\) J/mol K), F: 0.0614 (mp at 148.5°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C): 0.0974 (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)
0.0997; 0.0974 (supercooled liquid \(S_L\), GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.60 \(\times\) 10\(^{-5}\*) (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)
3.63 \(\times\) 10\(^{-4}\) (supercooled liquid \(P_L\), GC-RI correlation, Wang & Wong 2002)
\(\log (P_L/mmHg) = 48.01 – 6714/(T/K) – 12.028\cdot\log (T/K)\) (supercooled liquid \(P_L\), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa m\(^3\)/mol at 25°C): 1.48 (calculated-SOFA model, Govers & Krop 1998)
2.34, 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, \(\log K_{ow}\):
6.19 (calculated-SOFA model, Govers & Krop 1998)
6.31; 6.19 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Chlorinated Dibenzo-\(p\)-dioxins

Octanol/Air Partition Coefficient, log \(K_{OA}\):

Bioconcentration Factor, log BCF:
5.55 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log \(K_{OC}\):
6.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_\text{½}\):

Volatilization:

Photolysis:

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO_3}\) with NO\(_3\) radical and \(k_{O_3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:

\(k\) (oxidative degradation rate of water dissolved PCDD by ozone) is \(1.27 \times 10^6\) L g\(^{-1}\) min\(^{-1}\) under alkaline conditions at pH 10 and 20\(^\circ\)C (Palauschek & Scholz 1987)

\(k_{OH}(\text{calc}) = (21–22) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at room temp. (Atkinson 1991)

\(k_{OH} = (17–22) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\), calculated tropospheric lifetime \(\tau = 0.7–0.9\) d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of \(1.5 \times 10^6\) molecule/cm\(^3\) (Atkinson 1991)

\(k_{OH}(\text{calc}) = (4.5–5.9) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) with a calculated tropospheric lifetime \(\tau = 2.5–3.3\) d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime \(\tau = 0.7–0.9\) d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); the calculated tropospheric lifetime \(\tau = .5–3.3\) d for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone \(k = 1.27 \times 10^6\) L.g\(^{-1}\).min\(^{-1}\) under alkaline conditions at pH 10 and 20\(^\circ\)C (Palauschek & Scholz 1987).

Sediment:

Soil:

Biota:

<table>
<thead>
<tr>
<th>TABLE 8.1.1.8.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of 1,3,7-trichlorodibenzo-(p)-dioxin at various temperatures</td>
</tr>
<tr>
<td>Rordorf 1987, 1989</td>
</tr>
<tr>
<td>gas saturation-GC/ECD</td>
</tr>
<tr>
<td>(t/°C)</td>
</tr>
<tr>
<td>25</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>75</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>125</td>
</tr>
<tr>
<td>(\Delta H_v/(\text{kJ mol}^{-1}) = 86.4)</td>
</tr>
<tr>
<td>(\Delta H_{\text{subb}}/(\text{kJ mol}^{-1}) = 116.2)</td>
</tr>
<tr>
<td>(\Delta H_{\text{ fus}}/(\text{kJ mol}^{-1}) = 28.4)</td>
</tr>
</tbody>
</table>
FIGURE 8.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,7-trichlorodibenzo-p-dioxin.
8.1.1.9 2,3,7-Trichlorodibenzo-p-dioxin

Common Name: 2,3,7-Trichlorodibenzo-p-dioxin
Synonym: 2,3,7-TCDD
Chemical Name: 2,3,7-trichlorodibenzo-p-dioxin
CAS Registry No: 33857–28–2
Molecular Formula: \(\text{C}_{12}\text{H}_5\text{Cl}_3\text{O}_2\), \(\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2\)
Molecular Weight: 287.526
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
- Molar Volume (cm³/mol):
  - 179.11 (calculated-liquid density, Govers et al. 1990)
  - 239.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
- 88.2 (Rordorf 1987)
Enthalpy of Sublimation, \(\Delta H_{\text{subl}}\) (kJ/mol):
- 119.759 (Rordorf 1987)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
- 30.9 (Rordorf 1986, 1987)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), \(F\):

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0548 (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)
- 0.0674; 0.0548 (supercooled liquid \(S_L\), GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 0.000012* (calculated, Rordorf 1985a,b, 1986, 1987, 1989)
- 2.14 × 10⁻⁴ (supercooled liquid \(P_L\), GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

\[\log (P_L/\text{mmHg}) = 48.21 - 6829/(T/K) - 12.028 \log (T/K)\] (supercooled liquid \(P_L\), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 1.78 (calculated-SOFA model, Govers & Krop 1998)
- 2.04; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):
- 6.33 (calculated-SOFA model, Govers & Krop 1998)
- 6.46; 6.33 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Air Partition Coefficient, \(\log K_{\text{oa}}\) at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
- \(\log K_{\text{oa}} = -5.35 + 4320/(T/K)\) (generator column-GC/ECD, measured range 0–40°C, Harner et al. 2000)
- 9.42 (GC-retention time indices, Chen et al. 2002)
Bioconcentration Factor, log BCF:
5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_d:
7.05 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:
  Volatilization:
  Photolysis: photolysis rate k = 2.03 × 10^{-4} s^{-1} at 313 nm using a Hanovia 450-W mercury lamp in hexane solution (Dulin et al. 1986)
  Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
  k (oxidative degradation rate of water dissolved PCDD by ozone) is 1.27 × 10^6 L g^{-1} min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)
  k_{OH(calc)} = (21–22) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1991)
  k_{OH} = (17–22) × 10^{-12} cm^3 molecule^{-1} s^{-1}, calculated tropospheric lifetime τ = 0.7–0.9 d for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3 (Atkinson 1991)
  k_{OH(calc)} = (4.5–5.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} with a calculated tropospheric lifetime τ = 2.5–3.3 d for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

  Biodegradation:
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
  Air: tropospheric lifetime τ = 0.7 – 0.9 d calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);
  tropospheric lifetime τ(calc) = 2.5 – 3.3 d for the gas phase reaction with OH radical. (Kwok et al. 1995). Surface water:
  Groundwater: oxidative degradation rate of water dissolved PCDD by ozone k = 1.27 × 10^6 L·g^{-1}·min^{-1} under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987).

Sediment:
  Soil:
  Biota:

### TABLE 8.1.1.9.1
Reported vapor pressures and octanol-air partition coefficients of 2,3,7-trichlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Vapor pressure correlation</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Rordorf 1987, 1989</strong></td>
<td><strong>Harner et al. 2000</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>25</td>
<td>1.2 × 10^{-5}</td>
</tr>
<tr>
<td>50</td>
<td>5.2 × 10^{-4}</td>
</tr>
<tr>
<td>75</td>
<td>1.3 × 10^{-3}</td>
</tr>
<tr>
<td>100</td>
<td>0.21</td>
</tr>
<tr>
<td>125</td>
<td>2.3</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \Delta H_{fA}/(kJ \text{ mol}^{-1}) = 87.2 \]
\[ \Delta H_{sub}/(kJ \text{ mol}^{-1}) = 119.76 \]
\[ \Delta H_{ fus}/(kJ \text{ mol}^{-1}) = 30.9 \]

\[ \log K_{OA} = a + b/(T/K) \]
\[ a = -5.35 \]
\[ b = 4320 \]
\[ \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 82.7 \]
FIGURE 8.1.1.9.1 Logarithm of vapor pressure and $K_{OA}$ versus reciprocal temperature for 2,3,7-trichlorodibenzo-$p$-dioxin.
8.1.1.10 1,2,3,4-Tetrachlorodibenzo-p-dioxin

Common Name: 1,2,3,4-Tetrachlorodibenzo-p-dioxin
Synonym: 1,2,3,4-TCDD
Chemical Name: 1,2,3,4-tetrachlorodibenzo-p-dioxin
CAS Registry No: 30746–58–8
Molecular Formula: C_{6}H_{4}O_{2}C_{6}Cl_{4}
Molecular Weight: 321.971

Melting Point (°C):

Boiling Point (°C):
419 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
186.71 (calculated-liquid density, Govers et al. 1990)
186.10 (liquid molar volume, Govers et al. 1995)
260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆H_v (kJ/mol):
85.6 (Rordorf 1987)

Enthalpy of Sublimation, ∆H_{subl} (kJ/mol):
118.53 (Rordorf 1987)
111.3 (Li et al. 2004)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
31.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ∆S_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.0246 (mp at 189°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00063* (generator column-HPLC/UV, generator column-GC/ECD, Shiu et al. 1988)
0.00047* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988a)
S/(mol/L) = 2.75 × 10⁻¹⁰ exp(0.065·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
log x = -2447/(T/K) – 2.373, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
0.000388 (generator column-GC/MS, Santl et al. 1994)
ln x = –10.5076 – 3984/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0165 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.00 × 10⁻² (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
1.04 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)
6.30 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
6.37 × 10⁻⁴ (corrected supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1998)
2.48 × 10⁻⁴ (solid vapor pressure calculated from reported P_L, Delle Site 1997)
log (P/Pa) = 15.59851 – 6199.79/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
2.75 × 10⁻³ (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)
2.26 × 10⁻⁵ (solid Pₛ, gas saturation-GC/MS, Mader & Pankow 2003)
9.66 × 10⁻⁴ (supercooled liquid Pₗ, calculated from Pₛ assuming ΔSₙₛ = 56 J/mol K, Mader & Pankow 2003)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = 45.97 - 6777/(T/K) - 11.499 \log \left( \frac{P}{\text{K}} \right) \] (supercooled liquid Pₗ, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
\[ \ln \left( \frac{P}{\text{Pa}} \right) = 35.917 - 14276/(T/K), \text{ temp range 298–398 K} \] (regression eq. of Rordorf 1989 data, Li et al. 2004)
\[ \ln \left( \frac{P}{\text{Pa}} \right) = (33.217 ± 0.442) - (13386 ± 173)/(T/K); \text{ temp range 378–403 K} \] (Knudsen effusion technique, Li et al. 2004)

Henry’s Law Constant (Pa m³/mol at 25°C):
3.77 (calculated-P/C, Shiu et al. 1988)
2.02 (gas stripping-GC/MS, Santl et al. 1994)
3.02; 1.35 (quoted exp., calculated-SOFA model, Govers & Krop 1998)
1.15; 1.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log Kₐₜₕ:
8.65, 8.90, 8.96; 8.66, 8.91, 8.97 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
8.64, 8.91 (HPLC-RT correlation, Sarna et al. 1984)
8.63, 8.02; 8.64, 8.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
7.18, 7.08 (HPLC-RT correlation, Burkhard & Kuehle 1986)
6.20 (generator column-GC/ECD, Doucette & Andren 1987)
6.85 (HPLC-RT correlation, Doucette & Andren 1988b)
6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
7.18 (recommended, Sangster 1993)
7.18 (recommended, Hansch et al. 1995)
7.04 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log Kₐₜₕ at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
9.410 (calculated-Kₐₜₕ/Kₐₜₕ, Paterson et al. 1991)
9.70*; 9.86 (generator column-GC; calculated, Harner et al. 2000)
\[ \log K_{OA} = -4.96 + 4370/(T/K); \text{ temp range 10–40°C} \] (Harner et al. 2000)
9.64 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:
2.20, 3.40 (guppy, in whole fish, in lipid, Gobas et al. 1987)
2.90, 4.02 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log Kₜₕ:
7.88 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, tₕ:
Photolysis: solution photolysis tₜₙ = 1294 min in n-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis tₜₚ = 560 min on a clean glass surface under the same conditions (Nestrick et al. 1980)
sunlight induced photolysis tₜₚ = 380 min in isooctane solution and sunlight induced solid phase tₜₚ = 65 h
of TCDD dispersed as solid films (Buser 1988); photodegradation tₜₚ = 88 h for 1,2,3,4-TCDD adsorbed to clean silica gels in a rotary photo-reactor by filtered <290 nm of light (Koester & Hites 1992); first-order photodegradation k = 0.98 h⁻¹ with tₜₚ = 0.71 h when loaded on TiO₂ film under UV (λ > 300 nm) or solar light irradiation in the air (Choi et al. 2000)
Oxidation: rate constant k, for gas-phase second order rate constants, kₙₙ for reaction with OH radical, kₙₙ with NO₃ radical and kₙₙ with O₃ or as indicated. *data at other temperatures see reference: k (oxidative degradation rate of water dissolved PCDD by ozone) is 4.73 × 10⁵ L g⁻¹ min⁻¹ under alkaline condition at pH 10 and 20°C (Palaschek & Scholz 1987)
\[ k_{OH}(calc) = (16 - 19) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \] (Atkinson 1991)
\[ k_{\text{OH}} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] and a calculated tropospheric lifetime \( \tau = 0.8 - 2.0 \text{ d} \) based on gas phase OH reactions and a 12-h average daytime OH radical concentration of \( 1.5 \times 10^6 \text{ molecule/cm}^3 \) at room temp. (Atkinson 1991)

\[ k_{\text{OH}}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a calculated tropospheric lifetime \( \tau = 2.8 - 7.2 \text{ d} \) for a tri-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

\[ k_{\text{OH}} = 8.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 306 - 366 \text{ K (Brubaker & Hites 1997)} \]

\[ k_{\text{OH}}(\text{calc}) = 8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Brubaker & Hites 1998)} \]

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[ k_2 = 0.016 \text{ d}^{-1} \text{ (rainbow trout, Niimi & Oliver 1986)} \]

\[ k_1 = 953 \text{ d}^{-1}; k_2 = 1.20 \text{ d}^{-1} \text{ (guppy, Gobas & Schrap 1990)} \]

\[ k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 > 0.23 \text{ d}^{-1} \text{ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)} \]

\[ k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (average } k_1 \text{ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)} \]

Half-Lives in the Environment:

Air: tropospheric lifetime \( \tau = 0.802.0 \text{ d} \) calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime \( \tau = 2.8 - 7.2 \text{ d} \) for the gas phase reaction with OH radical (Kwok et al. 1995);

first-order photodegradation \( k = 0.98 \text{ h}^{-1} \) with \( t_{\text{hr}} = 0.71 \text{ h} \) when loaded on TiO\(_2\) film under UV (\( \lambda > 300 \text{ nm} \)) or solar light irradiation in the air (Choi et al. 2000).

Surface water: sunlight induced photolysis \( t_{\text{hr}} = 380 \text{ min} \) in isoctane min and \( t_{\text{hr}} = 65 \text{ h} \) dispersed as solid films (Buser 1988).

Groundwater:

Sediment: degradation \( t_{\text{hr}} = 20 - 200 \text{ yr} \) for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation \( t_{\text{hr}} = 10 - 100 \text{ yr} \) (estimated, Suzuki et al. 2000).

Biota: mean \( t_{\text{hr}} \approx 43 \text{ d} \) in rainbow trout (Niimi 1986);

biological \( t_{\text{hr}} = 43 \text{ d} \) in rainbow trout (Niimi & Oliver 1986);

biological \( t_{\text{hr}} = 5 - 14 \text{ d} \) in trout (Niimi 1987);

\( t_{\text{hr}} < 0.3 \text{ d} \) for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

### TABLE 8.1.1.10.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4-tetrachlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>( \log K_{OA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-HPLC/UV</td>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC/ECD</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>S/g·m(^{-3})</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>5</td>
<td>0.00034</td>
<td>4</td>
</tr>
<tr>
<td>15</td>
<td>0.00045</td>
<td>25</td>
</tr>
<tr>
<td>25</td>
<td>0.00063</td>
<td>40</td>
</tr>
<tr>
<td>35</td>
<td>0.00114</td>
<td>100</td>
</tr>
<tr>
<td>45</td>
<td>0.002085</td>
<td>125</td>
</tr>
<tr>
<td>( \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 46.8 ) ( 4 - 40 \text{ °C} )</td>
<td>( \Delta H_{vap}/(kJ \text{ mol}^{-1}) = 85.6 )</td>
<td>( \Delta H_{subl}/(kJ \text{ mol}^{-1}) = 118.53 )</td>
</tr>
</tbody>
</table>

\( \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 33.36 \) \( 5 - 45 \text{ °C} \)

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
FIGURE 8.1.1.10.1 Logarithm of mole fraction solubility, vapor pressure and KOA versus reciprocal temperature for 1,2,3,4-tetrachlorodibenzo-p-dioxin.
8.1.1.11  1,2,3,7-Tetrachlorodibenzo-p-dioxin

Common Name: 1,2,3,7-Tetrachlorodibenzo-p-dioxin
Synonym: 1,2,3,7-TCDD
Chemical Name: 1,2,3,7-tetrachlorodibenzo-p-dioxin
CAS Registry No: 67028–18–6
Molecular Formula: ClC₆H₃O₂C₆HCl₃
Molecular Weight: 321.971
Melting Point (°C):
  172–175  (Friesen et al. 1985)
Boiling Point (°C):
  438.3  (calculated, Rordorf 1987, 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  186.52  (calculated-liquid density, Govers et al. 1990)
  260.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
  90.9  (Rordorf 1987)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
  129.41  (Rordorf 1987)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
  36.6  (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
  25.31  (Friesen & Webster 1990)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
  82  (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming \( \Delta S = 56 \text{ J/mol K} \)), F: 0.0361 (mp at 172°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00042*  (20°C, ¹⁴C labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
0.00043*  (20°C, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)
0.00028  (20°C, ¹⁴C labeled, generator column-HPLC/LSC, Webster et al. 1986)
0.00048*  (21°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
0.0161; 0.0131  (supercooled liquid \( S_L \), GC-RI correlation, method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0 × 10⁻⁶*  (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1989)
7.0 × 10⁻⁶  (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
5.0 × 10⁻⁶  (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
2.69 × 10⁻⁵  (supercooled liquid \( P_L \), GC-RI correlation, Wang & Wong 2002)
\[ \log (P_l/\text{mmHg}) = 46.64 – 6978/(T/K) – 11.503\log (T/K) \]  (supercooled liquid \( P_L \), Kirchhoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa m³/mol at 25°C):
0.77  (calculated-P/C, Shiu et al. 1988)
1.78  (calculated-SOFA model, Govers & Krop 1998)
1.15; 1.48  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log $K_{ow}$:
8.19, 8.59, 8.81; 8.22, 8.60, 8.81 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
8.18, 8.60 (HPLC-RT correlation, Sarna et al. 1984)
8.15, 7.58; 8.19, 7.72 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
6.91 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
8.22 (recommended, Sangster 1993)
8.22 (recommended, Hansch et al. 1995)
7.05 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF:
3.17 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.44 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
3.44, 4.44 (fathead minnow, wet wt. based, lipid based, Gobas & Schrap 1990)
3.17, 4.17 (rainbow trout, wet wt. based, lipid based, Gobas & Schrap 1990)
3.18, 2.90 (rainbow trout, Opperhuizen & Sijm 1990)
3.30, 3.38 (fathead minnow, Opperhuizen & Sijm 1990)
3.09, 3.02–3.14; 3.35, 3.30–3.37 (rainbow trout, range; fathead minnow, range, De Voogt et al. 1990)
5.50 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{oc}$ at 25°C or as indicated:
4.26 (DOC, Muir et al. 1985)
5.39, 5.45, 5.59 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
5.98, 5.97, 5.91 (20, 30, 40°C, humic acid from peat bog, Webster et al. 1986)
6.55, 6.32, 6.44 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986)
7.87 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Vaporization:
Photolysis: $t_{1/2}$ = 563 min for solution photolysis in n-hexadecane at 1.0 m from a GE Model RS sunlamp and $t_{1/2}$ = 156 min for surface photolysis on a clean soft glass surface under the same conditions (Nestrick et al. 1980);
first order $k = 18.13 \times 10^{-6}$ s$^{-1}$ with $t_{1/2} = 0.069$ h in water-acetonitrile (2:3 v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 33.52 \times 10^{2}$ d$^{-1}$ with direct sunlight photolysis $t_{1/2} = 2.08$ d in spring, $k = 39.41 \times 10^{2}$ d$^{-1}$ with $t_{1/2} = 1.77$ d in summer, $k = 21.77 \times 10^{2}$ d$^{-1}$ with $t_{1/2} = 3.20$ d in autumn, $k = 12.86 \times 10^{2}$ d$^{-1}$ with $t_{1/2} = 8.73$ d in winter, in aquatic bodies at latitude 40°N and $t_{1/2} = 8.73$ d averaged over full year (Choudhary & Webster 1986, 1989).
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{oh}$ for reaction with OH radical, $k_{no}$ with NO$_3$ radical and $k_{o}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k$ (oxidative degradation rate of water dissolved PCDD by ozone) is $7.39 \times 10^{5}$ L g$^{-1}$ min$^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)
$k_{oh}(calc) = (16–19) \times 10^{12}$ cm$^{3}$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
$k_{oh} = (7.6–19) \times 10^{12}$ cm$^{3}$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime of 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^{6}$ molecule cm$^{-3}$ (Atkinson 1991)
$k_{oh}(calc) = (2.0–5.1) \times 10^{12}$ cm$^{3}$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation: rate constant $k = 0.096$ d$^{-1}$ for rainbow trout (Sijm et al. 1990).
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 317$ d$^{-1}$; $k_2 = 0.26$ d$^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)
$k_1 = 529 \text{ d}^{-1}$; $k_2 = 0.25 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985)

$k_2 = 0.178, 0.163 \text{ d}^{-1}$ (rainbow trout, fathead minnow exposed to dioxins in their diets, Muir & Yarechewski 1988; quoted, Opperhuizen & Sijm 1990; Sijm et al. 1990)

$k_1 = 420$ to $213 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.278$ to $0.250 \text{ d}^{-1}$ (rainbow trout exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)

$k_1 = 650$ to $408 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.322$ to $0.170 \text{ d}^{-1}$ (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)

$k_1 = 9.5 \times 10^{-2}, 19.1 \times 10^{-2} \text{ d}^{-1}$ (metabolic inhibitor PBO-treated rainbow trout, control fish, 2–21 d exposure: Sijm et al. 1990)

$k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 > 0.23 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish after 120-h exposure, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average $k_1$ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radical to be 0.8–2.0 d (Atkinson 1991); calculated tropospheric lifetime was 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 2.08 \text{ d}$ in spring, $t_{1/2} = 1.77 \text{ d}$ in summer, $t_{1/2} = 3.20 \text{ d}$ in fall, $t_{1/2} = 5.42 \text{ d}$ in winter, and $t_{1/2} = 8.73 \text{ d}$ averaged over a full year (Choudhary & Webster 1986);

$\Delta H_{sol} / (\text{kJ mol}^{-1}) = 50.68$

$25^\circ \text{C}$

$\Delta H_{fus} / (\text{kJ mol}^{-1}) = 36.6$

$25^\circ \text{C}$

$\Delta H_{subl} / (\text{kJ mol}^{-1}) = 129.41$

$25^\circ \text{C}$

$\Delta S_{fus} / (\text{J mol}^{-1} \text{K}^{-1}) = 82$

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
FIGURE 8.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,3,7-tetrachlorodibenzo-p-dioxin.
8.1.1.12 1,2,7,8-Tetrachlorodibenzo-p-dioxin

Common Name: 1,2,7,8-Tetrachlorodibenzo-p-dioxin
Synonym: 1,2,7,8-TCDD
Chemical Name: 1,2,7,8-tetrachlorodibenzo-p-dioxin
CAS Registry No: 34816–53–0
Molecular Formula: Cl₂C₆H₂O₂C₆H₂Cl₂
Molecular Weight: 321.971
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  186.88 (calculated-liquid density, Govers et al. 1990)
  260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/(mol K)):
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/(mol K)), F:
Water Solubility (g/m³ or mg/L at 25°C):
  0.000908 (supercooled liquid \( S_L \), calculated-SOFA model, Govers & Krop 1998)
  0.00223, 0.00908 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):
  4.37 × 10⁻³ (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998)
  4.17 × 10⁻³; 4.37 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
log (\( P_L/\text{mmHg} \)) = 46.50 – 6956/(T/K) – 11.503·log (T/K) (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa m³/mol at 25°C):
  1.48 (calculated-SOFA model, Govers & Krop 1998)
  1.29; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log \( K_{ow} \):
  6.38 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989a)
  6.99 (calculated-SOFA model, Govers & Krop 1998)
Octanol/Air Partition Coefficient, log \( K_{OA} \):
Bioconcentration Factor, log BCF:
  5.51 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)
Sorption Partition Coefficient, log \( K_{OC} \):
  7.99 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

**Volatilization:**

Photolysis: solution photolysis \( t_{1/2} = 491 \) min in \( n \)-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis \( t_{1/2} = 350 \) min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with \( NO_3 \) radical and \( k_{O_3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference: k (oxidative degradation rate of water dissolved PCDD by ozone) is \( 4.73 \times 10^5 \) L g\(^{-1}\) min\(^{-1}\) under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

\[
 k_{OH}(calc) = 7.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1991)}
\]

\[
 k_{OH} = (7.6–19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and a calculated tropospheric lifetime } \tau = 0.8–2.0 \text{ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of } 1.5 \times 10^6 \text{ molecule/cm}^3 \text{ (Atkinson 1991)}
\]

\[
 k_{OH}(calc) = (2.0–5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated tropospheric lifetime } \tau = 2.8–7.2 \text{ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)}
\]

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[
 k_1 = 38 \text{ L kg}^{-1} \text{ d}^{-1}; 49 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 > 0.9 \text{ d}^{-1}; > 0.3 \text{ d}^{-1} \text{ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)}
\]

\[
 k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (average } k_1 \text{ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)}
\]

Half-Lives in the Environment:

Air: tropospheric lifetime \( \tau = 0.8–2.0 \) d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

\[
 \text{tropospheric lifetime } \tau(calc) = 2.8–7.2 \text{ d for the gas-phase reaction with OH radical (Kwok et al. 1995)}.
\]

Surface water:

Groundwater:

Sediment: degradation \( t_{1/2} = 20–200 \) yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation \( t_{1/2} = 10–100 \) yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: \( t_{1/2} <0.7 \) d for PBO treated and \( t_{1/2} <2.1 \) d for control fish in 120-h exposure studies (Sijm et al. 1993).
8.1.1.13  1,3,6,8-Tetrachlorodibenzo-p-dioxin

Common Name: 1,3,6,8-Tetrachlorodibenzo-p-dioxin
Synonym: 1,3,6,8-TCDD
Chemical Name: 1,3,6,8-tetrachlorodibenzo-p-dioxin
CAS Registry No: 33423-92-6
Molecular Formula: Cl₄C₆H₄O₂C₆H₄Cl₂
Molecular Weight: 321.971
Melting Point (°C):
  219–219.5 (Pohland & Yang 1972; Rordorf 1987, 1989; Delle Site 1997)
Boiling Point (°C):
  438.3 (calculated, Rordorf 1987, 1989)
Density (g/cm³ at 20°C):
  192.34 (calculated-liquid density, Govers et al. 1990)
  260.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
  86.5 (Rordorf 1987)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
  125.793 (Rordorf 1987)
  118.6 (Li et al. 2004)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
  36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
  74 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming \( \Delta S = 56 \) J/mol K), F: 0.0125 (mp at 219°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.00032* (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)
  0.000317* (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
  0.000283, 0.000326, 0.000366, 0.000328 (¹⁴C-labeled/LSC, Milli-Q treated water, lake water, simulated lake water, Milli-Q water, Servos & Muir 1989a)
  0.0322 (supercooled liquid S₁, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.000537* (20°C, gas saturation, measured range 20–100°C, Webster et al. 1985)
  6.76 × 10⁻⁵ (supercooled liquid Pᵥ, GC-RI correlation, Wang & Wong 2002)
log (Pv/mmHg) = 46.99 – 6976/(T/K) – 11.503·log (T/K) (supercooled liquid Pᵥ, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
ln (P/Pa) = (35.818 ± 0.968) – (14262 ± 380)/(T/K), temp range 378–408 K (Knudsen effusion technique, Li et al. 2004)

Henry’s Law Constant (Pa m³/mol at 25°C):
  6.90 (23°C, batch stripping, Webster et al. 1985)
  3.77 (calculated-P/C, Shiu et al. 1988)
  1.15 (calculated-SOFA model, Govers & Krop 1998)
1.48; 1.15 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 8.72, 9.00, 9.42; 8.72, 9.02, 9.43 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 8.70, 9.02 (HPLC-RT correlation, Sarna et al. 1984)
- 8.70, 8.08; 8.70, 8.12 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 7.20, 7.13 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.13 (corrected HPLC-RT value, Burkhard & Kuehl 1986)
- 6.29 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
- 7.18 (recommended, Sangster 1993)
- 6.29 (recommended, Hansch et al. 1995)
- 6.79 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- 3.03, 2.67 (fathead minnow, rainbow trout, Corbet et al. 1983, 1988)
- 3.39 (rainbow trout, steady-state, wet weight basis, Muir et al. 1985)
- 3.83 (fathead minnow, steady-state, wet weight basis, Muir et al. 1985)
- 3.39, 3.83 (rainbow trout average, fathead minnow average, Muir et al. 1986)
- 1.08–3.75, 2.14, 1.76–1.93 (Amphipod in lake water, in simulated lake water, in water with Aldrich humic acid, Servos & Muir 1989a)
- 4.20, 4.20 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
- 5.00 (goldfish after 6 d exposure: metabolic inhibitor PBO-treated, Sijm et al. 1989b)
- 3.76, 3.54–3.90; 3.32, 3.23–3.40 (fathead minnow, range; rainbow trout, range, De Voogt et al. 1990)
- 3.83, 4.83 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
- 3.39, 4.39 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
- 3.46, 3.30, 3.15 (quoted, rainbow trout exposed to different concentrations, Opperhuizen & Sijm 1990)
- 3.76, 3.75 (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
- 3.70 (10.1 ng/L for 0–10 d, predicted for biota held in lake enclosures, Sijm et al. 1992b)
- 3.12 (17.7 ng/L for 0–10 d, invertebrates, Sijm et al. 1992b)
- 3.20 (21.4 ng/L for 0–10 d, unionid clams & white suckers gill, Sijm et al. 1992b)
- 2.36 (3.1 ng/L for 0–10 d, white suckers carcass, Sijm et al. 1992b)
- 2.31 (1.6 ng/L for 14–24 d, invertebrates, Sijm et al. 1992b)
- 2.95 (0.9 ng/L for 14–24 d, unionid clams, Sijm et al. 1992b)
- 3.32 (2.1 ng/L for 14–24 d, white suckers gill, Sijm et al. 1992b)
- 2.70 (1.0 ng/L for 14–24 d, white suckers carcass, Sijm et al. 1992b)
- 4.54 (3.5 ng/L for 0–104 d, white suckers gill, Sijm et al. 1992b)
- 4.26 (1.8 ng/L for 0–104 d, white suckers carcass, Sijm et al. 1992b)
- 3.13 (gold fish, PBO-treated, 120-h exposure, Sijm et al. 1993)
- 5.53 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{OC}$:
- 4.36 (DOC, De Voogt et al. 1990)
- 6.74 (calculated-$K_{OW}$, Corbet et al. 1988)
- 2.11–3.75, 2.39, 2.05–2.38 (DOC partition coeff., lake water, simulated lake water, Aldrich humic acid, Servos & Muir 1989a)
- 5.98–6.23 (sediment, Servos & Muir 1989b)
- 7.50 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 6.23 (derived from soot-water distribution coeff., Bärring et al. 2002)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$, or Lifetimes, $\tau$:
- Volatilization: 3.9 d in water of 0.5 m depth in a small pond (Corbet et al. 1988)
Photolysis: solution photolysis \( t_{1/2} = 507 \) min in \( n \)-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis on a clean glass surface under the same conditions with \( t_{1/2} = 264 \) min (Nestrick et al. 1980; quoted, Muto et al. 1991);

first-order \( k = 59.57 \times 10^{-6} \) s\(^{-1}\) in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: \( t_{1/2} = 0.35 \) d in spring, \( t_{1/2} = 0.31 \) d in summer, \( t_{1/2} = 0.53 \) d in fall, \( t_{1/2} = 0.84 \) d in winter and \( t_{1/2} = 1.47 \) d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)

\( t_{1/2} = 14.0–28.5 \) h in outdoor pool and \( t_{1/2} = 6.3–8.0 \) d in natural water in a Pyrex flask under sunlight (Corbet et al. 1988)

\( t_{1/2} = 25 \) h in water column (Corbet et al. 1983)

\( t_{1/2} = 6.3–8.0 \) d for natural water under sunlight and photodegradation \( t_{1/2} = 0.3 \) d in summer sunlight at 40°N and \( t_{1/2} = 7 \) d in a 1-L flask (Corbet et al. 1988)

photolysis \( k = 59.57 \times 10^{-6} \) s\(^{-1}\) with \( t_{1/2} = 3.24 \) h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: \( k = 198.13 \times 10^{-2} \) d\(^{-1}\) with \( t_{1/2} = 0.35 \) d in spring, \( k = 226.99 \times 10^{-2} \) d\(^{-1}\) with \( t_{1/2} = 0.31 \) d in summer, \( k = 130.91 \times 10^{-2} \) d\(^{-1}\) with \( t_{1/2} = 0.53 \) d in fall, \( k = 82.85 \times 10^{-2} \) d\(^{-1}\) with \( t_{1/2} = 0.84 \) d in winter; while experimentally determined sunlight photolysis \( t_{1/2} = 3.5 \) d for \(^{14}C\) labeled 1,3,6,8-TCDD in pond water (Choudhary & Webster 1989)

\( t_{1/2} = 78.8 \) h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, *data at other temperatures see reference: photooxidation may be an important path of transformation (Corbet et al. 1988)

\( k \) (oxidative degradation rate of water dissolved PCDD by ozone) is \( 3.21 \times 10^5 \) L g\(^{-1}\) min\(^{-1}\) under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

\( k_{OH}(calc) = (16–19) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at room temp. (Atkinson 1991)

\( k_{OH} = (7.6–19) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) and a calculated tropospheric lifetime \( \tau = 0.8–2.0 \) d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of \( 1.5 \times 10^6 \) molecule cm\(^{-3}\) at room temp. (Atkinson 1991)

\( k_{OH}(calc) = (2.0–5.1) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) with a calculated tropospheric lifetime \( \tau = 2.8–7.2 \) d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Biocaccumulation, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\( k_1 = 184 \) d\(^{-1}\); \( k_2 = 0.10 \) d\(^{-1}\) (rainbow trout, flow-through system, Muir et al. 1985)

\( k_1 = 574 \) d\(^{-1}\); \( k_2 = 0.10 \) d\(^{-1}\) (fathead minnow, Muir et al. 1985; quoted, Adams et al. 1986)

\( k_1 = 225, 221, 106 \) d\(^{-1}\) (rainbow trout fry, exposed to concn of 4, 74, 211 ng/L, 5-d uptake study, Muir et al. 1986)

\( k_1 = 0.074, 0.110, 0.111 \) d\(^{-1}\) (rainbow trout fry, exposed to 4, 74, 211 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

\( k_1 = 526, 621 \) d\(^{-1}\) (fathead minnow, exposed to concn of 10, 41 ng/L, 5-d uptake study, Muir et al. 1986)

\( k_1 = 0.08, 0.122 \) d\(^{-1}\) (fathead minnow, exposed to concn of 10, 41 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

\( k_1 = 225, 97 \) L kg\(^{-1}\) d\(^{-1}\) (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

\( k_1 = 0.211 \) d\(^{-1}\) (fathead minnow, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

\( k_1 = 0.158 \) d\(^{-1}\) (rainbow trout, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

\( k_1 = 225, 221, 106 \) mL g\(^{-1}\) d\(^{-1}\); \( k_2 = 0.074, 0.110, 0.110 \) d\(^{-1}\) (rainbow trout exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

\( k_1 = 526, 621 \) mL g\(^{-1}\) d\(^{-1}\); \( k_2 = 0.080, 0.122 \) d\(^{-1}\) (fathead minnow exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

\( k_1 = 1200 \) d\(^{-1}\); \( k_2 = 0.06 \) d\(^{-1}\) (filter-feeder, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

\( k_1 = 285 \) d\(^{-1}\); \( k_2 = 0.12 \) d\(^{-1}\) (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)
k_1 = 142, 116 L kg^{-1} d^{-1}; k_2 = 0.14, > 0.24 d^{-1} (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k_1 = 66 L kg^{-1} d^{-1}, 104 L kg^{-1} d^{-1} (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime \( \tau = 0.8–2.0 \) d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction rate with OH radicals (Atkinson 1991);
calculated tropospheric lifetime \( \tau = 2.8–7.2 \) d for with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis in aquatic bodies at latitude 40°N for various seasons with half-lives: 0.35 d in spring, 0.31 d in summer, 0.53 d in fall, 0.84 d in winter and 1.47 d averaged over full year (Choudhary & Webster 1986);

\( t_{1/2} = 14.0–28.5 \) h for outdoor pool and \( t_{1/2} = 6.3–8.0 \) d for natural water in a Pyrex flask under sunlight (Corbet et al. 1988);

\( t_{1/2} = 3.24 \) h for photolysis in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude calculated to be: \( t_{1/2} = 0.35 \) d in spring, \( t_{1/2} = 0.31 \) d in summer, \( t_{1/2} = 0.53 \) d in fall, and \( t_{1/2} = 0.84 \) d in winter (Choudhary & Webster 1989); calculated transformation rate constant in simulated lake enclosure of 9.4 \( \times \) 10^{-2} h^{-1} (Servos et al. 1992a).

Groundwater:

Sediment: \( t_{1/2} = 51.2–69.2 \) d (Corbet et al. 1988);
calculated \( t_{1/2} = 10 \) yr with a transformation rate constant \( k = 7.9 \times 10^{-6} \) h^{-1} (Servos et al. 1992a);
degradation \( t_{1/2} = 20–200 \) yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation \( t_{1/2} = 10–100 \) yr (estimated, Suzuki et al. 2000).

Biota: \( t_{1/2} = 4 \) d in rainbow trout (Neely 1979; quoted, Niimi & Oliver, 1983, 1986);

\( t_{1/2} = 4 \) d in rainbow trout (Corbet et al. 1983; quoted, Niimi & Oliver 1986);

\( t_{1/2} = 2 \) d in rainbow trout (Muir et al. 1984);

\( t_{1/2} = 6–9 \) d for both rainbow trout fry and fathead minnow (Muir et al. 1986);

\( t_{1/2} = 6.90 \) d in fathead minnow (Adams et al. 1986);

\( t_{1/2} = 41 \) to 44 d in rooted vegetable (Corbet et al. 1988);

\( t_{1/2} = 15 \) d in whole body of rainbow trout (Muir et al. 1990);

half-lives in gold fish: \( t_{1/2} = 4.8 \) d for PBO treated and \( t_{1/2} < 0.3 \) d for control fish in 120-h exposure studies (Sijm et al. 1993)

---

**TABLE 8.1.1.13.1**

Reported aqueous solubilities and vapor pressures of 1,3,6,8-tetrachlorodibenzo-\( p \)-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Webster et al. 1985</strong></td>
<td><strong>Rordorf 1987, 1989</strong></td>
</tr>
<tr>
<td>generator column-HPLC/LSC</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/g \cdot m^{-3} )</td>
</tr>
<tr>
<td>20</td>
<td>( 3.20 \times 10^{-4} )</td>
</tr>
<tr>
<td>40</td>
<td>( 3.90 \times 10^{-3} )</td>
</tr>
<tr>
<td>( \Delta H_{v}/(kJ \ mol^{-1}) = 86.5 )</td>
<td>( \Delta H_{ub}/(kJ \ mol^{-1}) = 125.794 )</td>
</tr>
</tbody>
</table>
FIGURE 8.1.1.13.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,3,6,8-tetrachlorodibenzo-\(p\)-dioxin.
8.1.1.14 1,3,7,8-Tetrachlorodibenzo-\(p\)-dioxin

![Structure of 1,3,7,8-Tetrachlorodibenzo-\(p\)-dioxin]

Common Name: 1,3,7,8-Tetrachlorodibenzo-\(p\)-dioxin  
Synonym: 1,3,7,8-TCDD  
Chemical Name: 1,3,7,8-tetrachlorodibenzo-\(p\)-dioxin  
CAS Registry No: 50585–46–1  
Molecular Formula: \(\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2\)  
Molecular Weight: 321.971  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm\(^3\) at 20°C):  
188.33 (calculated-liquid density, Govers et al. 1990)  
260.6 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):  
88.9 (Rordorf 1987)  
Enthalpy of Sublimation, \(\Delta H_{\text{subl}}\) (kJ/mol):  
127.77 (Rordorf 1987)  
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):  
36.6 (Rordorf 1987)  
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):  
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), \(F\):  
Water Solubility (g/m\(^3\) or mg/L at 25°C):  
0.0203 (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)  
0.0223, 0.0203 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):  
8.4 \times 10^{-7}, 4.5 \times 10^{-5}, 1.4 \times 10^{-3}, 2.6 \times 10^{-2}, 0.35 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)  
8.32 \times 10^{-3} (supercooled liquid \(P_L\), calculated-SOFA model, Govers & Krop 1998)  
4.17 \times 10^{-4}; 8.32 \times 10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
log \(\left(\frac{P_L}{\text{mmHg}}\right) = 46.80 - 6977/(T/K) - 11.503\log (T/K) \) (supercooled liquid \(P_L\), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)  
Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):  
1.26 (calculated-SOFA model, Govers & Krop 1998)  
1.29; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):  
6.80 (calculated-SOFA model, Govers & Krop 1998)  
6.93; 6.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
6.30; 6.29, 6.28, 6.40, 6.44 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

$5.52$ (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

$7.72$ (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis: solution photolysis $t_{1/2} = 153$ min in $n$-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 160$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{1/2} = 86.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with $OH$ radical, $k_{NO3}$ with $NO_3$ radical and $k_{O3}$ with $O_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = 13 \times 10^{-12}$ cm$^3$ molecule$^{-1}$·s$^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6 - 19) \times 10^{-12}$ cm$^3$ molecule$^{-1}$·s$^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8-2.0$ d based on gas phase $OH$ reactions and a 12-h average daytime $OH$ radical concentration of $1.5 \times 10^6$ molecule cm$^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(calc) = (2.0 - 5.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$·s$^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8-7.2$ d at for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 57$ L kg$^{-1}$ d$^{-1}$; $99$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.14$ d$^{-1}$; $> 0.24$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish. 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66$ L kg$^{-1}$ d$^{-1}$, $104$ L kg$^{-1}$ d$^{-1}$ (average $k_1$ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8-2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with $OH$ radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8-7.2$ d for the gas-phase reaction with $OH$ radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20-200$ yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10-100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 2.1$ d for PBO treated and $t_{1/2} < 0.4$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
8.1.1.15  1,3,7,9-Tetrachlorodibenzo-p-dioxin

Common Name: 1,3,7,9-Tetrachlorodibenzo-p-dioxin
Synonym: 1,3,7,9-TCDD
Chemical Name: 1,3,7,9-tetrachlorodibenzo-p-dioxin
CAS Registry No: 62470–53–5
Molecular Formula: Cl₄C₆H₂O₂C₆H₂Cl₂
Molecular Weight: 321.971
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  192.34  (calculated-liquid density, Govers et al. 1990)
  260.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
  123.6   (Li et al. 2004)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  0.0294   (supercooled liquid \( S_L \), calculated-SOFA model, Govers & Krop 1998)
  0.0294, 0.0294 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  5.50 \times 10^{-5}  (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998)
  5.89 \times 10^{-5}; 5.50 \times 10^{-5}  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
  \log (P_L/mmHg) = 46.86 – 6956/(T/K) – 11.503\log (T/K)  (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
  \ln (P/Pa) = (37.221 \pm 0.469) – (14864 \pm 185)/(T/K); temp range 383–408 K  (Knudsen effusion technique, Li et al. 2004)
Henry’s Law Constant (Pa m³/mol at 25°C):
  0.589   (calculated-SOFA model, Govers & Krop 1998)
  1.42; 0.589  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log \( K_{OW} \):
  6.39  (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)
  6.68  (calculated-SOFA model, Govers & Krop 1998)
  6.83; 6.68  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
  6.28, 6.12, 6.47, 6.44  (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)
Octanol/Air Partition Coefficient, log \( K_{OA} \):
Bioconcentration Factor, log BCF:
  5.67   (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)
Sorption Partition Coefficient, log \( K_{OC} \):
  7.51   (sediment/water, calculated-SOFA model, Govers & Krop 1998)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

**Volatileization:**
- Photolysis: solution photolysis $t_{1/2} = 499$ min in $n$-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 169$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)
- $t_{1/2} = 79.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}(\text{calc}) = (16 - 19) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (7.6 - 19) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8 - 2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6$ molecule cm$^{-3}$ at room temp. (Atkinson 1991)
- $k_{OH}(\text{calc}) = (2.0 - 5.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8 - 7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 54$ L kg$^{-1}$ d$^{-1}$, 98 L kg$^{-1}$ d$^{-1}$; $k_2 < 0.1$ d$^{-1}$, > 2.1 d$^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 66$ L kg$^{-1}$ d$^{-1}$, 104 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

**Air:** tropospheric lifetime $\tau = 0.8 - 2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8 - 7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

**Surface water:**

**Groundwater:**

**Sediment:** degradation $t_{1/2} = 20 - 200$ yr for all homologues (estimated, Suzuki et al. 2000).

**Soil:** degradation $t_{1/2} = 10 - 100$ yr (estimated, Suzuki et al. 2000).

**Biota:** half-lives in gold fish: $t_{1/2} > 7$ d for PBO treated and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
8.1.1.16 2,3,7,8-Tetrachlorodibenzo-\(p\)-dioxin

Common Name: 2,3,7,8-Tetrachlorodibenzo-\(p\)-dioxin
Synonym: 2,3,6,7-tetrachlorodibenzo-\(p\)-dioxin, TCDD, TCDBD, 2,3,6,7- TCDD, 2,3,7,8-TCDD, dioxin
Chemical Name: 2,3,7,8-tetrachlorodibenzo-\(p\)-dioxin
CAS Registry No: 1746–01–6
Molecular Formula: \(\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2\)
Molecular Weight: 321.971
Melting Point (°C):
295  (Lide 2003)
Boiling Point (°C):
421.2  (Schroy et al. 1985a)
Density (g/cm\(^3\) at 20°C):
1.827  (solid at 25°C, Boer et al. 1972; Schroy et al. 1985a)
1.021  (liquid at normal boiling point, Schroy et al. 1985a)
Molar Volume (cm\(^3\)/mol):
184.32, 184.97  (calculated-liquid density, crystalline volume, Govers et al. 1990)
188.34  (liquid molar volume, Govers et al. 1990)
260.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
71.71  (at normal bp, Schroy et al. 1985a)
79.9  (Rordorf 1987)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
123.91  (Schroy et al. 1985b)
124.001  (Rordorf 1987)
Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
38.91  (Boer et al. 1972; Schroy et al. 1985a,b; Ruelle & Kesselring 1997)
38.9, 36.6  (Obs., predicted, Rordorf 1986, 1987)
Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{ fus} = 56\) J/mol K), F: 0.00244 (mp at 295°C)
0.0017  (Shiu et al. 1988)
4.07 \times 10^{-4}  (calculated, Passivirta et al. 1999)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0002  (shake flask-GC/ECD, Crummett & Stehl 1973)
3.17 \times 10^{-4}  (\(^{14}\text{C}-\text{labeled, generator column-HPLC/LSC, Webster et al. 1983})
1.93 \times 10^{-5}  (shake flask-GC/MS, Marple et al. 1986a)
7.91 \times 10^{-6}  (\(^{14}\text{C}-\text{labeled, Adams & Blaine 1986})
1.29 \times 10^{-4}, 4.83 \times 10^{-4}  (4.3, 17.3°C, generator column-GC/MS, Lodge 1989)
\log [S_s/(mol/L)] = 0.190–2089/(T/K)  (supercooled liquid, Passivirta et al. 1999)
0.0158  (supercooled liquid S_s, GC-RI correlation, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0 \times 10^{-7}  (\(^{14}\text{C}-\text{gas saturation method, Jaber & Podoll 1983})
(4.50 \pm 2) \times 10^{-6}  (\text{gas saturation-GC, Rordorf 1985a})
(3.5–6.3) \times 10^{-6}, (1.3–3.1) \times 10^{-5}, (2.8–8.9) \times 10^{-5}, (3.9–15.9) \times 10^{-5}, (4.4–21.9) \times 10^{-5}  (25, 50, 75, 100, 125°C, predicted using estimated \(\Delta H_{ subl}\) and \(\Delta S_{ subl}\) for tetra-chloro isomers, Rordorf 1985a)
4.61 \times 10^{-3}*  (30.1°C, gas saturation-GC/MS, measured range 30.1–71.1°C Schroy et al. 1985a,b)
\log (P/mmHg) = 12.89784 – 6477.132/(273.15 + t/°C); temp range 10–305°C (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)
\[
\log (P/\text{mmHg}) = 8.78307 - 4098.173/(273.15 + t/°C); \text{ temp range 305–420°C (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)}
\]
\[
2.02 \times 10^{-7}*, 4.60 \times 10^{-7}, 9.65 \times 10^{-6}, 4.58 \times 10^{-5}, 1.59 \times 10^{-4} (25, 30, 62, 71°C, results derived from Antoine eq., gas saturation-GC/MS, Schroy et al. 1985b)
\]
\[
\ln (P/\text{Pa}) = 34.570834 - \left[\frac{14903.438}{(T/K)}\right], \text{ temp range: 28 3.15–578.15 K (gas saturation, Schroy et al. 1985a)}
\]
\[
\ln (P/\text{Pa}) = 25.104351 - 93430.391/(T/K), \text{ temp range: 578.15–703.15 K (gas saturation, Schroy et al. 1985a)}
\]
\[
8.71 \times 10^{-6} (20°C, gas saturation-LSC, measured range 20–100°C, Webster et al. 1985)
\]
\[
9.87 \times 10^{-8} (\text{14C-gas saturation, Podoll et al. 1986})
\]
\[
8.14 \times 10^{-5}, 6.0 \times 10^{-5}, 9.7 \times 10^{-5}; 1.1 \times 10^{-4} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
\]
\[
\]

Henry’s Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations):

\[
0.0021 \quad (\text{calculated-P/C, Mabey et al. 1982})
\]
\[
0.152 \quad (\text{calculated-P/C, Crosby 1985})
\]
\[
0.212 \quad (\text{calculated-P/C, Schroy et al. 1985})
\]
\[
1.64 \quad (\text{calculated-P/C, Podoll et al. 1986})
\]
\[
1.63, 3.34, 10.34 (\text{calculated-P/C, Shiu et al. 1988})
\]
\[
7.93 \quad (\text{calculated-P/C, Jury et al. 1990})
\]
\[
1.62 \quad (\text{calculated-SOFA model, Govers & Krop 1998})
\]
\[
\log [H/(Pa m³/mol)] = 8.86–1574/(T/K) (Passivirta et al. 1999)
\]
\[
1.12; 1.62 (\text{GC-RI correlation; calculated-SOFA, Wang & Wong 2002})
\]

Octanol/Water Partition Coefficient, log K_{OW}:

\[
5.38 \quad (\text{Crummett & Stehl 1973})
\]
\[
6.19 \quad (\text{Neely 1979; Veith et al. 1979; Corbet et al. 1983})
\]
\[
6.15 \quad (\text{Kenaga 1980})
\]
\[
8.93 \quad (\text{HPLC-RT correlation, Sarna et al. 1984})
\]
\[
7.02 \quad (\text{HPLC-RT correlation, Burkhard & Kuehl 1986})
\]
\[
6.64 \quad (\text{shake flask-GC/MS, Marple et al. 1986b})
\]
\[
6.42 \quad (\text{shake flask/slow stirring method-GC/MS, Sijm et al. 1989a})
\]
\[
7.02 \quad (\text{recommended, Sangster 1993})
\]
\[
6.53 \quad (\text{recommended, Hansch et al. 1995})
\]
\[
7.06 \quad (\text{GC-RI correlation, Wang & Wong 2002})
\]

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

\[
9.70 \quad (\text{calculated-K_{OW}/K_{AW}, Wania & Mackay 1996})
\]
\[
10.05*; 9.91 (\text{generator column-GC; calculated, Harner et al. 2000})
\]
\[
11.04 (7°C, GC-retention time correlation, Harner et al. 2000)
\]
\[
\log K_{OA} = -6.19 + 4840/(T/K); \text{ temp range 10–50°C (generator column-GC/ECD, Harner et al. 2000)}
\]
\[
9.95 (\text{GC-retention time indices correlation, Chen et al. 2002})
\]
Bioconcentration Factor, log BCF:

1.69, 2.34, 2.08 (daphnia, ostracod, brine shrimp, 14C-labeled-LSC, Matsumura & Benezet 1973)
4.30–4.41; 3.6–3.95 (snail, gambusia, daphnids; duckweed, algae, catfish; Isensee & Jones 1975)
3.96 (rainbow trout, Branson et al. 1985)
3.90 (fathead minnow, steady-state, wet weight, Adams et al. 1986)
3.73, 4.55 (fish: flowing water test, static ecosystem test, Kenaga & Goring 1980, Kenaga 1980)
3.97 (rainbow trout, Branson et al. 1983)
3.97, 3.67 (rainbow trout: whole body, muscle, Branson et al. 1985)
1.38–1.60 (rhesus monkey, Geyer et al. 1986)
4.11 (guppy, Oppenhaizen et al. 1986)
4.43, 4.59 (rainbow trout: measured average, estimated BCF at steady-state, for 28-d exposure, Mehrle et al. 1988)
4.30, 5.0 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
3.89, 4.59 (fathead minnow, rainbow trout, De Voogt et al. 1990)
5.80, 5.90 (goldfish after 6 d exposure: PBO-treated, control, Sijm et al. 1989b)
4.11, 5.64 (guppy, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.97, 4.70; 4.97, 5.70 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
4.63, 4.40 (pine needle/air BCF values, Reissinger et al. 1989)
4.59, 4.58, 4.93, 4.57, 3.97 (rainbow trout, quoted, Oppenhaizen & Sijm 1990)
4.11, 3.90, 3.78 (guppy, fathead minnow, mosquito fish, quoted, Oppenhaizen & Sijm 1990)
2.62 (human, Webster & Connett 1991)
5.24; 4.91 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
5.24; 4.83; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-C<sub>f</sub>/C<sub>w</sub>; calculated; rate constant ratio k<sub>1</sub>/k<sub>2</sub> from non-linear regression analysis, Loonen et al. 1994b)
5.24; 5.48 (lipid wt. base, quoted exp., calculated-SOFA model, Govers & Krop 1998)
5.71, 6.71 (fish medeka 10% lipid: BCF<sub>p</sub>, BCF<sub>L</sub>, Geyer et al. 2000)
6.02, 6.05 (fish muscle log BCF<sub>L</sub> calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K<sub>OC</sub>:

5.67 (organic carbon soil, calculated-K<sub>OC</sub> Ow, Kenaga 1980)
6.95, 7.39–7.58 (calculated-K<sub>OC</sub> Ow, 10 soils from Missouri & New Jersey, Jackson et al. 1985)
6.22–6.54; 5.96–6.09 (red clay soil from Missouri, Alluvial soil from Missouri, Marple et al. 1986)
4.83 (hydroxy aluminum-clay, Srinivasan & Fogler 1987)
6.60 (14C-labeled, soil, batch equilibrium-sorption isotherm, GC/ECD, Walters & Guiseppi-Elie 1988)
3.06 (soil, Eduljee 1987)
6.30; 7.59; 7.25 (Lake Ontario sediment; solids; DOC dissolved organic carbon; batch equilibrium-sorption isotherm, Lodge & Cook 1989)
6.24, 6.10, 5.10 (Eglin Air Force Base soil/water with 0.01% surfactant from Florida at pH 4, 7, 8.5, batch equilibrium-GC, Puri et al. 1989)
6.50, 5.86, 4.81 (Time Beach soil/water with 0.01% surfactant from Missouri at pH 4, 7, 8.5, Puri et al. 1989)
5.70, 5.09, 4.76 (Visalia soil/water with 0.01% surfactant from California at pH 4, 7, 8.5, Puri et al. 1989)
6.44, 6.66 (batch equilibrium-sorption isotherms: 2-d, 10-d isotherm, regression analysis for sorption of uncontaminated Time Beach soil from water, Walters et al. 1989)
6.14 (soil, Jury et al. 1990)
6.80 (Baltic sea particulate filed samples, concn distribution-GC/MS, Broman et al. 1991)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization: probably not an important process (Callahan et al. 1979)

\[ t_{1/2} = 20–200 \text{ d from water column which will be slowed down further by the fact that it is sorbed to the sediment and biota (Mill 1985)} \]
\[ t_{1/2} \sim 32 \text{ d for ponds and } t_{1/2} \sim 16 \text{ d for rivers (Podoll et al. 1986)} \]
\[ t_{1/2} = 104 \text{ d from soil by calculation assuming diffusion of TCDD in soil is vapor-dominated up to volumetric water content of 0.3 m}^3/^3, \text{ and then liquid-dominated to saturation (Eduljee 1987)} \]
\[ t_{1/2} = 190 \text{ d (Thibodeaux & Lipsky 1985; quoted, Eduljee 1987)} \]
t½ = 365 d for volatilization from below surface soil (Jury et al. 1990)
k = 0.0054 h⁻¹ with t½ = 128 h from grass foliage (McCrady & Maggard 1993)

Photolysis:

stable to sunlight for at least 14 d in distilled water (Crosby et al. 1971; quoted, Dougherty et al. 1991)
t½ = 3 h in methanol solution in sunlight (Plimmer et al. 1973)
t½ = 56 min for vapor in sunlight (Peterson 1976; quoted, Mill 1985)
thin film of TCDD on glass plates showed transformation at about 6 h (Crosby & Wong 1977; quoted, Mill 1985)
t½ = 56.8 min in n-hexadecane on a clean soft glass surface at 1.0 m from a GE Model RS sunlamp and surface photolysis t½ = 140 h on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984; Dougherty et al. 1991)

TCDD extracted from the aqueous sludge with hexane can be continuously degraded by a mercury arc of UV radiation (Exner et al. 1982; quoted, Crosby 1985)
t½ ~ 1 d in water, t½ = 0.1 d in vapor and t½ = 1–100 d in soil with t½ = 50 d for a small fraction in water column in equilibrium with sediment sorbed with TCDD (Mill 1985)
kₚ = 6.94 × 10⁻⁶ s⁻¹ with t½ = 27 h as a 90:10 mixture of distilled water and acetonitrile under summer sunlight; kₚ = 0.15 d⁻¹ with t½ = 6 d in summer sunlight at 40°L surface waters (Dulin et al. 1986)
t½ = 81 h after adjusting for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
k = 0.14 d⁻¹ with t½ = 118 h in winter, k = 0.61 d⁻¹ with t½ = 27 h in spring, k = 0.78 d⁻¹ in summer, and k = 0.32 d⁻¹ with t½ = 51 h in autumn for aqueous dissolved TCDD in sunlight over four seasons at 40°N latitude (Nestrick et al. 1980; quoted, Mamantov 1984; Dougherty et al. 1991)

photodegradation t½ = 10 min, a very rapid process at soil surface during the day (Facchetti et al. 1986)
t½ = 14 min sunlight induced photolysis in isooctane solution and sunlight induced solid phase t½ = 300 h dispersed as solid films (Buser 1988)
k = 5.9 × 10⁻³ s⁻¹ rate constant for photolysis in air at 150–350°C (Orth et al. 1989)
k = 0.15 min⁻¹ first-order photolysis rate constant in isooctane and over 90% was lost in 21 min of irradiation in isooctane whereas only greater than 55% TCDD remained in soil after 15 d of irradiation (Kieatiwong et al. 1990)

photolytic degradation t½ = 4.5 h in extract from fly ash exposed to UV light from a distance of 20 cm for native congener and t½ = 5.2 h for 13C-labeled congener in tetracene solution (Tysklind & Rappe 1991)
t½ = 31 min in hexadecane and t½ = 27 min in ethyl oleate (Dougherty et al. 1991)
photodegradation k = 0.0156 h⁻¹ with t½ = 44 h for TCDD sorbed to grass foliage and exposed to natural sunlight (McCrady & Maggard 1993)
t½ = 52 h, direct sunlight photolysis in water-acetonitrile in midday of mid-summer at 40°N (quoted, Zepp 1991)
t½ = 55.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, k₉⁻ for reaction with OH radical, k₉₀ with NO₃ radical and k₉₀ with O₃ or as indicated, *data at other temperatures see reference:
k = 6 × 10⁻⁷ s⁻¹ with t½ = 320 h, estimated for the reaction with 3 × 10⁻¹⁵ mole OH radicals in vapor phase (Singh 1977; quoted, Mill 1985)
laboratory tests shown that 99.5% TCDD was oxidized in 21 s at 800°C while only 50% reacted at 700°C (Esposito et al. 1980; quoted, Crosby 1985)
k₀₉ = 2 × 10⁸ mol⁻¹ s⁻¹ with t½ = 13 d for oxidation in vapor phase (Mill 1985)
k₀₉ >1.0 × 10⁸ mol⁻¹ s⁻¹, 1.7 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ with t½ = 200 h (Podoll et al. 1986)
k₀₉(calc) = 9 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with an atmospheric lifetime τ ~ 3 d (Atkinson 1987a)
k₀₉(calc) = 8.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship Atkinson 1987b)
photooxidation t½ = 22.3–223 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
k = 1.33 × 10² L g⁻¹ min⁻¹, the oxidative degradation of water dissolved TCDDs by ozone takes place only under alkaline conditions at pH 10 and 20°C (Palacshek & Scholz 1987)
k₀₉(calc) = 7.6 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)
k₀₉(calc) = (7.6 - 19) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ and a calculated tropospheric lifetime τ = 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 × 10⁶ molecule/cm³ at room temp. (Atkinson 1991)
k₀₉(calc) = 4 × 10⁸ M⁻¹ s⁻¹ in aqueous solutions (Haag & Yao 1992)
k_{OH(calc)} = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated tropospheric lifetime } \tau = 2.8–7.2 \text{ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)}

Hydrolysis: hydrolysis is not likely under environmental conditions (Callahan et al. 1979; Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:
- $t_{1/2(aq.\text{aerobic})} = 10032 \text{ h, based on soil die-away test data (Kearney et al. 1971; quoted, Howard et al. 1991)}$
- and $t_{1/2} = 14160 \text{ h, based on lake water and sediment dieaway test data (Ward & Matsumura 1978; quoted, Howard et al. 1991)}$
- $t_{1/2} > 1.0 \text{ yr (Callahan et al. 1979)}$
- $t_{1/2(aq.\text{anaerobic})} = 40128–56640 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}$

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (estimated, Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 4.64 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 5.00 \times 10^{-4} \text{ h}^{-1}$ (rainbow trout, Neely 1979)
- $k_1 = 108 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.012 \text{ d}^{-1}$ (rainbow trout, Branson et al. 1983, 1985)
- $k_1 = 476 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.120 \text{ d}^{-1}$ (fathead minnow, Adams et al. 1986)
- $k_1 = 600 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (guppy, Oppenhuizen et al. 1986)
- $k_1 = 1832, 1543, 1337, 1591 \text{ d}^{-1}$ and $k_2 = 0.047, 0.041, 0.015, 0.043 \text{ d}^{-1}$ (rainbow trout, exposed to 38 pg/L, 176 pg/L, 382 pg/L, 702 pg/L for 28 d, Mehrle et al. 1988)
- $k_1 = 216, 604 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)
- $k_1 = 0.008 \text{ d}^{-1}$ (rainbow trout, quoted, Oppenhuizen & Sijm 1990)
- $k_1 = 381 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.048 \text{ d}^{-1}$ (fathead minnow, quoted, Oppenhuizen & Sijm 1990)
- $k_1 = 100 \text{ mL g}^{-1} \text{ d}^{-1}$ (mosquito fish, quoted, Oppenhuizen & Sijm 1990)
- $k_1 = 86 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish, 120-h exposure, metabolic inhibitor PBO-treated; Sijm et al. 1993)
- $k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, 104 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 > 1.3 \text{ d}^{-1}$; < 0.1 d$^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated; control, Sijm et al. 1993)
- $k_1 = 500 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.049 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)
- $k_1 = 0.0061 \text{ d}^{-1}$ with a biological $t_{1/2} = 49 \text{ d}$ (blue mussel, 99-d exposure, Heikotein et al. 1994)
- $k_1 = 0.0246 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)
- $k_1 = 0.0199 \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: dominant transformation process in the atmosphere (Atkinson et al. 1982)
- $t_{1/2} = 200 \text{ h for reaction with OH radical (Podoll et al. 1986)}$
- atmospheric lifetime of ~3 d at room temp. (Atkinson 1987a)
- $t_{1/2} = 22.3–223 \text{ h, based on estimated photooxidation half-life in air (Howard et al. 1991)}$
- $t_{1/2} = 1 \text{ h, an upper limit, undergo rapid photolysis in vapor phase (Travis & Hattemer-Frey 1987)}$
- atmospheric k = 0.012 min$^{-1}$ with $t_{1/2} = 58 \text{ min in summer sunlight at 40°N latitude (Buser 1988)}$
- reaction rate constant k ~ 0.02 h$^{-1}$ (Paterson et al. 1990)
- tropospheric lifetime $\tau(calc) = 0.8–2.0 \text{ d for reaction with OH radical (Atkinson 1991)}$
- tropospheric lifetime $\tau(calc) = 2.8–7.2 \text{ d for with OH radical (Kwok et al. 1995)}$
- $t_{1/2} = 200 \text{ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000)}$

Surface water: photolysis $t_{1/2} = 3 \text{ h in methanol solution under sunlight (Plimmer et al. 1973)}$
- $t_{1/2} = 600 \text{ d in a model aquatic environment (Ward & Matsumura 1978)}$
- reaction rate constant estimated to be $2.6 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985)
- calculated sunlight photolysis half-lives over four seasons at 40°N latitude averaged over for 24 h exposure per day: $t_{1/2} = 130 \text{ h in winter, } t_{1/2} = 28 \text{ h in spring, } t_{1/2} = 20 \text{ h in summer and } t_{1/2} = 52 \text{ h in fall (Mill et al. 1982; quoted, Mill 1985)}$
- calculated photolysis half-lives in sunlight at 40°N latitude: $t_{1/2} = 118 \text{ h in winter, } t_{1/2} = 27 \text{ h in spring, } t_{1/2} = 21 \text{ h in summer and } t_{1/2} = 51 \text{ h in fall (Podoll et al. 1986)}$
- photolysis $t_{1/2} = 40 \text{ h in near-surface waters is an important degradative pathway (Travis & Hattemer-Frey 1987)}$
- $t_{1/2} = 14 \text{ min, sunlight-induced photolysis half-life in isooctane (Buser 1988)}$
- reaction rate constant estimated to be 0.008 h$^{-1}$ (Paterson et al. 1990);
photolysis $t_{1/2} = 27–81$ h, aerobic $t_{1/2} = 1.15–1.62$ yr, anaerobe $t_{1/2} = 4.58–6.45$ yr (Howard et al. 1991)

$t_{1/2} = 4000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passiivirta 2000).

Groundwater: $t_{1/2} = 20064–28320$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 12000–14400$ h in aquatic sediment (Ward & Matsumura 1978; quoted, Quensen & Matsumura 1983)

reaction rate constant $k \approx 8.0 \times 10^{-6}$ h$^{-1}$ (Mackay et al. 1985)

$k \approx 1.5 \times 10^{-5}$ h$^{-1}$ (Paterson et al. 1990)

t$_{1/2} > 1$ yr (O’Keefe et al. 1986)

t$_{1/2} = 9.9–98$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000)

$900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passiivirta 2000).

Soil: $t_{1/2} = 10032–14160$ h, based on soil dieaway test data for two soils (Howard et al. 1991);

t$_{1/2} \approx 1$ yr (Kearney et al. 1973; quoted, Quensen & Matsumura 1983);

degradation $t_{1/2} = 10–12$ yr in soil (De Dimenico et al. 1980, Kimbrough et al. 1984);

t$_{1/2} \approx 1$ yr if applied to surface on soil with 2,4-D (Nash & Beall 1980);

$k \approx 8.0 \times 10^{-6}$ h$^{-1}$ (Mackay et al. 1985)

$k \approx 1.1 \times 10^{-5}$ h$^{-1}$ (Paterson et al. 1990)

t$_{1/2} = 10$ min during the day, photodegradation is a rapid process at the soil surface (Facchetti et al. 1986);

t$_{1/2} \approx 10$ yr if TCDD is on or near the surface and $t_{1/2} = 100$ yr if TCDD is buried at greater depth

(Nauman & Schaum 1987)

calculated $t_{1/2} = 10$ yr (Eduljee 1987)

t$_{1/2} = 10$ yr or longer (Boddington et al. 1990)

t$_{1/2} = 365$ d for volatilization to atmosphere below surface soil (Jury et al. 1990)

t$_{1/2} = 10$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 10–100$ yr in soils (estimated, Suzuki et al. 2000)

$900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passiivirta 2000).

Biota: $t_{1/2} = 31$ d, estimated half-life in rat (Rose et al. 1976; quoted, Birnbaum 1985);

t$_{1/2} = 11$ d, estimated half-life in hamster (Olsen et al. 1980; quoted, Birnbaum 1985)

t$_{1/2} = 30$ d, estimated half-life in guinea pig (Decad et al. 1981a; quoted, Birnbaum 1985)

t$_{1/2} = 11–24$ d, estimated half-life in mouse (Gasiewicz et al. 1983; quoted, Birnbaum 1985)

depuration $t_{1/2} = 58$ d, total body burden of 14C-TCDD in whole rainbow trout (Branson et al. 1983, 1985)

t$_{1/2} = 17–37$ d in mouse, $t_{1/2} = 31$ d in rat and $t_{1/2} = 30$ d in guinea pig (quoted, Van den Berg et al. 1985)

elimination $t_{1/2} = 14.5$ d from fathead minnow (Adams et al. 1986)

t$_{1/2} = 105$ d in whole body of rainbow trout (Kleeman et al. 1986);

$300–325$ d in carp (Kuehl et al. 1986)

biological $t_{1/2} = 58$ d for rainbow trout (Niimi & Oliver 1986)

t$_{1/2} = 5.8$ yr in human (estimated, Poiger & Schlatter 1986)

t$_{1/2} > 336$ d for humans in Lake Superior (Kuehl et al. 1987)

elimination $t_{1/2} = 15–48$ d from rainbow trout for exposures of different concn (Mehrle et al. 1988)

$7.1$ yr in human (estimated, Pirkle et al. 1989; quoted, Webster & Connett 1991)

t$_{1/2} = 5 – 8$ yr for human, $t_{1/2} = 17.4–31$ d for rats, $t_{1/2} = 9.6–24.4$ d for mice, $t_{1/2} = 22–93.7$ d for guinea pigs,

$12.0–150$ d for hamsters, $t_{1/2} = 1$ yr for monkeys (Boddington et al. 1990)

$40.3$ d for lactating cows (Olling et al. 1991)

$5 – 10$ yr assumed half-life for human (Schecter & Ryan 1991)

elimination $t_{1/2} = 35–37$ d from lake trout sac fry (Walker et al. 1991)

$4.4$ yr for a 70 kg non-lactating “reference” human (Webster & Connett 1991)

t$_{1/2} < 0.5$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

elimination $t_{1/2} = 45$ d from soft-shell clam (Brown et al. 1994)

biological $t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994)

reported $t_{1/2} = 8–24.4$ d for mice, $t_{1/2} = 30.2$ and 93.7 d for guinea pigs, $t_{1/2} = 20–28.9$ d for rats and $t_{1/2} = 365–3470$ d for humans (Miniero et al. 2001).

depuration $t_{1/2} = 28$ d for newly contaminated oysters, and $t_{1/2} = 35$ d for chronically contaminated oysters (Gardinelli et al. 2004)
TABLE 8.1.1.16.1
Reported vapor pressures of 2,3,7,8-tetrachlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.1</td>
<td>4.61 × 10^{-7}</td>
<td>30</td>
<td>4.67 × 10^{-7}</td>
<td>20</td>
<td>8.71 × 10^{-6}</td>
<td>25</td>
<td>2.0 × 10^{-7}</td>
</tr>
<tr>
<td>30.2</td>
<td>5.19 × 10^{-7}</td>
<td>54.6</td>
<td>1.83 × 10^{-5}</td>
<td>50</td>
<td>1.12 × 10^{-5}</td>
<td>50</td>
<td>9.5 × 10^{-6}</td>
</tr>
<tr>
<td>30.3</td>
<td>8.73 × 10^{-7}</td>
<td>62</td>
<td>4.97 × 10^{-5}</td>
<td>100</td>
<td>1.72 × 10^{-5}</td>
<td>75</td>
<td>2.6 × 10^{-4}</td>
</tr>
<tr>
<td>54.6</td>
<td>2.06 × 10^{-5}</td>
<td>71</td>
<td>1.59 × 10^{-4}</td>
<td>100</td>
<td>4.6 × 10^{-3}</td>
<td>100</td>
<td>9.5 × 10^{-6}</td>
</tr>
<tr>
<td>55</td>
<td>1.37 × 10^{-5}</td>
<td>125</td>
<td>5.7 × 10^{-2}</td>
<td>125</td>
<td>5.7 × 10^{-2}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.2</td>
<td>1.94 × 10^{-5}</td>
<td>54.6</td>
<td>2.06 × 10^{-5}</td>
</tr>
<tr>
<td>55.2</td>
<td>3.71 × 10^{-5}</td>
<td>71</td>
<td>1.58 × 10^{-4}</td>
</tr>
<tr>
<td>61.9</td>
<td>4.58 × 10^{-4}</td>
<td>71.1</td>
<td>1.59 × 10^{-4}</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.1</td>
<td>12.89784</td>
<td>30</td>
<td>273.15</td>
</tr>
<tr>
<td>30.2</td>
<td>6477.132</td>
<td>50</td>
<td>273.15</td>
</tr>
<tr>
<td>30.3</td>
<td>6477.132</td>
<td>75</td>
<td>273.15</td>
</tr>
<tr>
<td>54.6</td>
<td>6477.132</td>
<td>100</td>
<td>273.15</td>
</tr>
<tr>
<td>55</td>
<td>6477.132</td>
<td>125</td>
<td>273.15</td>
</tr>
</tbody>
</table>

FIGURE 8.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-p-dioxin.
### TABLE 8.1.1.16.2
Reported octanol-air partition coefficients of 2,3,7,8-tetrachlorodibenzo-p-dioxin at various temperatures

Harner et al. 2000

generator column-GC/ECD

<table>
<thead>
<tr>
<th>t/°C</th>
<th>K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>10.318</td>
</tr>
<tr>
<td>40</td>
<td>9.283</td>
</tr>
<tr>
<td>50</td>
<td>8.778</td>
</tr>
<tr>
<td>25</td>
<td>10.05</td>
</tr>
</tbody>
</table>

\[
\log K_{OA} = a + b/(T/K)
\]

| a    | -6.19 |
| b    | 4840  |

enthalpy of phase change
\[ \Delta H_{OA}/(kJ \, mol^{-1}) = 92.60 \]

![Logarithm of K_{OA} versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-p-dioxin.](image)

**FIGURE 8.1.16.2** Logarithm of \( K_{OA} \) versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-p-dioxin.
8.1.1.17 1,2,3,4,7-Pentachlorodibenzo-p-dioxin

Common Name: 1,2,3,4,7-Pentachlorodibenzo-p-dioxin
Synonym: 1,2,3,4,7-P5CDD
Chemical Name: 1,2,3,4,7-pentachlorodibenzo-p-dioxin
CAS Registry No: 39227–61–7
Molecular Formula: ClC₆H₃O₂C₆Cl₄
Molecular Weight: 356.416
Melting Point (°C): 195 (Lide 2003)
Boiling Point (°C): 464.7 (calculated, Rordorf 1987, 1989)
Density (g/cm³ at 20°C):
- 197.74 (calculated-liquid density, Govers et al. 1990)
- 281.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
- 92.8 (Rordorf 1987)
Enthalpy of Sublimation, ΔHₘₜ (kJ/mol):
- 137.419 (Rordorf 1987)
Enthalpy of Fusion, ΔH₋₃ (kJ/mol):
- 42.4 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
- 26 (Friesen & Webster 1990)
Entropy of Fusion, ΔS₋₃ (J/mol K):
- 90 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming ΔS₋₃ = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
- 0.000118*; 0.0000855 (20°C, ¹⁴C-labelled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)
- 0.0000955 (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1986)
- 1.23 × 10⁻⁴⁺ (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
- 0.00428 (supercooled liquid Sₗ, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 8.80 × 10⁻⁸⁺ (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987,1989)
- 1.00 × 10⁻⁶ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
- 1.00 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- log (P/Pa) = 17.02207 – 7179.05/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 4.57 × 10⁻⁶ (supercooled liquid Pₗ, GC-RI correlation; Wang & Wong 2002)

Henry’s Law Constant (Pa m³/mol at 25°C):
- 0.264 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
- 0.224; 1.23 (supercooled liquid Pₗ, quoted expl., calculated-SOFA model, Govers & Krop 1998)
- 0.691; 1.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- $9.44, 9.62, 10.02; 9.39, 9.65, 10.05$ (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- $9.40, 9.65$ (HPLC-RT correlation, Sarna et al. 1984)
- $9.48, 8.80; 9.40, 8.64$ (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- $9.65, 7.44$ (HPLC-RT correlation, Burkhard & Kuehl 1986)
- $6.60$ (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
- $9.40, 9.65$ (HPLC-RT correlation, Sarna et al. 1984)
- $9.48, 8.80; 9.40, 8.64$ (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- $9.65, 7.44$ (HPLC-RT correlation, Burkhard & Kuehl 1986)
- $6.60$ (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
- $10.67^*$; $10.32$ (generator column-GC; calculated, Harner et al. 2000)
- $\log K_{OA} = -7.65 + 5460/(T/K)$, temp range 30–50°C (Harner et al. 2000)
- $10.42$ (GC-retention time correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:
- $3.26$ (fathead minnow, steady-state, wet weight, Muir et al. 1985)
- $2.50$ (rainbow trout, steady-state, wet weight, Muir et al. 1985)
- $3.16, 2.91$ (fathead minnow, rainbow trout, De Voogt et al. 1990;)
- $3.50, 4.50$ (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
- $5.37$ (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
- $4.85, 4.60, 4.50$ (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986b)
- $5.80, 5.67, 5.90$ (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986b)
- $6.38, 6.39, 6.46$ (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
- $5.02$ (DOC, De Voogt et al. 1990)
- $8.57$ (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- **Vaporization:** rate constant $k = 4.31 \times 10^{-6}$ s$^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated half-lives under conditions of variable sunlight intensity at 4°N latitude: $t_{1/2} = 18.29$ d in spring with rate constant $k = 0.466 \times 10^{-6}$ s$^{-1}$, $t_{1/2} = 15.16$ d in summer with $k = 0.562 \times 10^{-6}$ s$^{-1}$, $t_{1/2} = 28.59$ d in fall with $k = 0.298 \times 10^{-6}$ s$^{-1}$, $t_{1/2} = 52.37$ d in winter with $k = 0.163 \times 10^{-6}$ s$^{-1}$, and $t_{1/2} = 76.82$ d averaged over full year with rate constant $k = 0.111 \times 10^{-6}$ s$^{-1}$ (Choudhary & Webster 1985a, 1986); $k = 4.3115 \times 10^{-6}$ s$^{-1}$ in water-acetonitrile (3:3 v/v) at 313 nm (Choudhary & Webster 1985b); photolysis $k = 4.31 \times 10^{-6}$ s$^{-1}$ with $t_{1/2} = 45.86$ h in water-acetonitrile (2.3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 4.03 \times 10^2$ d$^{-1}$ with $t_{1/2} = 18$ d in spring, $k = 4.86 \times 10^2$ d$^{-1}$ with $t_{1/2} = 15$ d in summer, $k = 2.58 \times 10^2$ d$^{-1}$ with $t_{1/2} = 29$ d in fall, $k = 1.41 \times 10^2$ d$^{-1}$ with $t_{1/2} = 52$ d in winter (Choudhary & Webster 1989); $k = 0.74$ d$^{-1}$ under mid-summer sunlight at 50°N latitude in filtered-sterilized natural water and $k = 0.058$ d$^{-1}$ in (2.3, v/v) distilled water-acetonitrile (Friesen et al. 1990); photolytic $t_{1/2} = 38$ h in fly-ash extract (Tysklind & Rappe 1991); $t_{1/2} = 92$ h for photodegradation in a rotary photoreactor adsorbed to clean silica gel by filtered <290 nm of light (Koester & Hites 1992).

- **Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  $k_{OH}(calc) = (12 – 14) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
  $k_{OH} = (6.5 – 14) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1–2.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6$ molecule cm$^{-3}$ at room temp. (Atkinson 1991)
  $k_{OH}(calc) = (1.7 – 3.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0–8.5$ d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation: biotransformation rate constant \( k = 0.014 \, \text{d}^{-1} \) for rainbow trout (Sijm et al. 1990).

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:
- \( k_1 = 285 \, \text{d}^{-1};\, k_2 = 0.22 \, \text{d}^{-1} \) (fathead minnow, flow-through system, Muir et al. 1985)
- \( k_1 = 204 \, \text{d}^{-1};\, k_2 = 0.28 \, \text{d}^{-1} \) (rainbow trout, flow-through system, Muir et al. 1985)
- \( k_1 = 2.5 \times 10^{-2},\, 3.9 \times 10^{-2} \, \text{d}^{-1} \) (rainbow trout for 2 to 21 d exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1990)
- \( k_1 = 509,\, 162 \, \text{L} \, \text{kg}^{-1} \, \text{d}^{-1};\, k_2 < 0.1,\, > 1.5 \, \text{d}^{-1} \) (goldfish after 120-h exposure for metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- \( k_1 = 169 \, \text{L} \, \text{kg}^{-1} \, \text{d}^{-1},\, 251 \, \text{L} \, \text{kg}^{-1} \, \text{d}^{-1} \) (average \( k_1 \) for \( P_5 \text{CDD} \) homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
- Air: tropospheric lifetime of 1.1–2.4 d calculated for the gas-phase with OH radicals using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm^3, (Atkinson 1991);
- photodegradation \( t_{90} = 92 \, \text{h} \) in a rotary photo-reactor adsorbed to clean silica gel by filtered \( \lambda < 290 \, \text{nm} \) of light (Koester & Hites 1992);
- calculated tropospheric lifetime of 4.0–8.5 d for penta-chlorinated dioxin for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);
- suggested \( t_{90} = 200 \, \text{h} \) at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile solution \((4:6, \text{v/v})\): \( t_{90} = 18.29 \, \text{d} \) in spring, \( t_{90} = 15.16 \, \text{d} \) in summer, \( t_{90} = 28.6 \, \text{d} \) in fall, \( t_{90} = 52.37 \, \text{d} \) in winter, and \( t_{90} = 76.82 \, \text{d} \) averaged over full year (Choudhary & Webster 1985a, 1986);
- photolysis \( t_{90} = 45.86 \, \text{h} \) in water-acetonitrile \((2.3, \text{v/v})\) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: \( t_{90} = 18.4 \, \text{d} \) in spring, \( t_{90} = 15 \, \text{d} \) in summer, \( t_{90} = 29 \, \text{d} \) in fall and \( t_{90} = 52 \, \text{d} \) in winter (Choudhary & Webster 1989);
- \( t_{90} = 27 \, \text{d} \) in sunlit surface water and \( t_{90} = 0.94 \, \text{d} \) in surface water of actual pond (Friesen et al. 1990).

Groundwater:
- Sediment: degradation half-lives in sediment 20–200 yr for all homologues (estimated, Suzuki et al. 2000).
- Soil: degradation half-lives in soil 10–100 yr (estimated, Suzuki et al. 2000).
- Biota: \( t_{90} = 3.1 \, \text{d} \) in fathead minnow (Adams et al. 1986);
- \( t_{90} = 2 \, \text{d} \) in whole body of rainbow trout (Muir & Yarechewski 1988);
- half-lives in gold fish: \( t_{90} > 7 \, \text{d} \) for PBO treated and \( t_{90} < 0.5 \, \text{d} \) for control fish in 120-h exposure studies (Sijm et al. 1993).

### TABLE 8.1.1.17.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7-pentachlorodibenzo-\( p \)-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log ( K_{OA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Generator</strong></td>
<td><strong>Correlation</strong></td>
<td><strong>Log ( K_{OA} )</strong></td>
</tr>
<tr>
<td><strong>Column-HPLC/LSC</strong></td>
<td><strong>Column-GC/ECD</strong></td>
<td><strong>Saturation Pressure</strong></td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>**S/g·m(^{-3})</td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>20</td>
<td>1.20 × 10(^{-4})</td>
<td>7</td>
</tr>
<tr>
<td>40</td>
<td>3.17 × 10(^{-4})</td>
<td>11.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21</td>
</tr>
<tr>
<td></td>
<td></td>
<td>26</td>
</tr>
<tr>
<td></td>
<td></td>
<td>41</td>
</tr>
</tbody>
</table>

\( \log K_{OA} = a + b/(T/K) \)
TABLE 8.1.17.1 (Continued)

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>$\log K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Friesen et al. 1985</strong></td>
<td><strong>Friesen &amp; Webster 1990</strong></td>
<td><strong>Rordorf 1987, 1989</strong></td>
</tr>
<tr>
<td>generator column-HPLC/LSC</td>
<td>generator column-HPLC/LSC</td>
<td>vapor pressure correlation</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>7–41 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\Delta H_{sol}/(kJ \cdot mol^{-1}) = 47.5$

$7–41 °C$

**FIGURE 8.1.17.1** Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 1,2,3,4,7-pentachlorodibenzo-$p$-dioxin.
8.1.1.18 1,2,3,7,8-Pentachlorodibenzo-\(p\)-dioxin

![Chemical Structure](image)

Common Name: 1,2,3,7,8-Pentachlorodibenzo-\(p\)-dioxin
Synonym: 1,2,3,7,8-P5CDD
Chemical Name: 1,2,3,7,8-pentachlorodibenzo-\(p\)-dioxin
CAS Registry No: 40321–76–4
Molecular Formula: \(\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{HCl}_3\)
Molecular Weight: 356.416
Melting Point (°C): 464.7  
Boiling Point (°C):  
Density (g/cm\(^3\) at 20°C):  
Molar Volume (cm\(^3\)/mol): 195.74  
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 88.7 (Rordorf 1987)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol): 134.062 (Rordorf 1987)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol): 42.4 (Rordorf 1987)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K): 83 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), \(F\): 0.000722 (calculated, Passivirta et al. 1999)

Water Solubility (g/m\(^3\) or mg/L at 25°C and the reported temperature dependence equations):  
9.82 × 10\(^{-5}\) (calculated-QSAR, Fielder & Schramm 1990)  
2.77 × 10\(^{-3}\) (supercooled liquid \(S_L\), quoted exptl., calculated-SOFA model, Govers & Krop 1998)  
\[\log \left[\frac{S_L}{(\text{mol/L})}\right] = 0.445 - 2232/(T/K)\] (supercooled liquid, Passivirta et al. 1999)  
4.0 × 10\(^{-3}\); 2.77 × 10\(^{-3}\) (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):  
5.80 × 10\(^{-8}\) (calculated, Rordorf 1985a,b, 1987,1989; quoted, Kaupp & McLachlan 1999)  
1.20 × 10\(^{-5}\) (supercooled liquid \(P_L\), quoted exptl., calculated-SOFA model, Govers & Krop 1998)  
1.71 × 10\(^{-4}\); 1.23 × 10\(^{-7}\) (supercooled liquid \(P_L\); converted to solid \(P_S\) with fugacity ratio \(F\), Passivirta et al. 1999)  
\[\log \left(\frac{P_L}{(\text{Pa})}\right) = 12.72 - 5850/(T/K)\] (solid, Passivirta et al. 1999)  
\[\log \left(\frac{P_S}{(\text{Pa})}\right) = 8.38 - 3321/(T/K)\] (supercooled liquid, Passivirta et al. 1999)  
4.17 × 10\(^{-6}\); 1.20 × 10\(^{-5}\) (supercooled liquid \(P_L\); GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C and the reported temperature dependence equations):  
1.48 (calculated-SOFA model, Govers & Krop 1998)  
\[\log \left(\frac{H}{(\text{Pa} \text{ m}^3/\text{mol})}\right) = 7.94 - 1089/(T/K)\] (Passivirta et al. 1999)  
0.661; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log \(K_{ow}\):  
6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989a)  
7.50 (calculated-SOFA model, Govers & Krop 1998)  
7.27 (estimated-solubility \(S_L\) and regression eq. using lit. \(K_{ow}\) values, Passivirta et al. 1999)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 7.215 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.55; 7.50 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
- 6.78, 6.84, 6.49, 6.87 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

- 10.57*; 10.44 (generator column-GC; calculated, Harner et al. 2000)
- 11.63 (7°C, GC-retention time correlation, Harner et al. 2000)
- log $K_{OA} = -8.02 + 5540/(T/K)$; temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
- 10.46 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log $BCF$:

- Bioconcentration Factor, log $BCF$:
  - 3.20 (guppy, exposed to fly ash extract, Opperhuizen et al. 1986)
  - 3.93; 4.31 (goldfish: PBO treated; control, 120-h exposure, Sijm et al. 1993)
  - 5.27 (guppies, 21-d exposure, system-I absence of sediment, Loonen et al. 1994b)
  - 4.98 (guppies, 21-d exposure, system-II with sediment, Loonen et al. 1984b)
  - 5.34 (calculated-SOFA model, Govers & Krop 1998)

- 3.20 (guppy, exposed to fly ash extract, Opperhuizen et al. 1986)
- 6.78, 6.84, 6.49, 6.87 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Sorption Partition Coefficient, log $K_{OC}$:

- 6.80 (Baltic sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)
- 8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization:
  - Photolysis: solution photolysis $t_{1/2} = 456$ min in $n$-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 52.8$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);
  - photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{1/2} = 33.6$ h for native congener and $t_{1/2} = 16.7$ h for $^{13}$C-labeled congener in tetradeacne solution (Tysklind & Rappe 1991);
  - $t_{1/2} = 57.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures see reference:
  - $k_{OH(calc)} = 6.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
  - $k_{OH} = (6.5 - 14) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1$–2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6$ molecule cm$^{-3}$ at room temp. (Atkinson 1991)
  - $k_{OH(calc)} = (1.7 - 3.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0$–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

- Hydrolysis:

- Biodegradation:

- Biotransformation:

- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 700$ mL g$^{-1}$ d$^{-1}$; $k_2 = 0.090$ d$^{-1}$ (guppy, Opperhuizen et al. 1986)
  - $k_1 = 127, 695$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.02, < 0.1$ d$^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)
  - $k_1 = 169$ L kg$^{-1}$ d$^{-1}$, 251 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
  - $k_1 = 952$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.030$ d$^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)
  - $k_2 = 0.0051$ d$^{-1}$ with $t_{1/2} = 50$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

- Half-Lives in the Environment:

  - Air: for a penta-chlorinated dioxin, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$, the tropospheric lifetime $\tau = 1.1$–2.4 d for the gas phase with OH radical (Atkinson 1991);
calculated tropospheric lifetime $\tau = 4.0–8.5$ d for reaction with OH radical (Kwok et al. 1995); $t_{1/2} = 360$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 7200$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Groundwater:

Sediment: $t_{1/2} = 1000000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: $t_{1/2} = 1,000,000$ h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000);

degradation $t_{1/2} = 10–100$ yr in soil (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 32$ d for PBO treated and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

**TABLE 8.1.18.1**

| Vapor pressure correlation | log $K_{OA}$
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>P/Pa</td>
</tr>
<tr>
<td>25</td>
<td>$5.8 \times 10^{-8}$</td>
</tr>
<tr>
<td>50</td>
<td>$3.8 \times 10^{-6}$</td>
</tr>
<tr>
<td>75</td>
<td>$1.4 \times 10^{-4}$</td>
</tr>
<tr>
<td>100</td>
<td>$3.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>125</td>
<td>$4.6 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

$\Delta H_v/(kJ \text{ mol}^{-1}) = 88.7$

$\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 138.062$

$\Delta H_{fus}/(kJ \text{ mol}^{-1}) = 42.4$

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 106$

for GC-RT correlation

**FIGURE 8.1.18.1** Logarithm of vapor pressure and $K_{OA}$ versus reciprocal temperature for 1,2,3,7,8-pentachlorodibenzo-$p$-dioxin.

© 2006 by Taylor & Francis Group, LLC

© 2006 by Taylor & Francis Group, LLC
8.1.1.19 1,2,4,7,8-Pentachlorodibenzo-p-dioxin

Common Name: 1,2,4,7,8-Pentachlorodibenzo-p-dioxin
Synonym: 1,2,4,7,8-P5CDD
Chemical Name: 1,2,4,7,8-pentachlorodibenzo-p-dioxin
CAS Registry No: 58802–08–7
Molecular Formula: Cl_2C_6H_2O_2C_6HCl_3
Molecular Weight: 356.416
Melting Point (°C): 206 (Rordorf 1987)
Boiling Point (°C): 464.7 (calculated, Rordorf 1987, 1989)
Density (g/cm³ at 20°C): 199.91 (calculated-liquid density, Govers et al. 1990)
281.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol): 91.8 (Rordorf 1987)
Enthalpy of Sublimation, ΔH_subl (kJ/mol): 136.636 (Rordorf 1987)
125.3 (Li et al. 2004)
Enthalpy of Fusion, ΔH_fus (kJ/mol): 42.4 (Rordorf 1987)
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.0168 (mp at 206°C)
Water Solubility (g/m³ or mg/L at 25°C): 9.82 × 10⁻³ (calculated-QSAR, Fielder & Schramm 1990)
4.92 × 10⁻³ (supercooled liquid S_L, quoted expl., calculated-SOFA model, Govers & Krop 1998)
5.39 × 10⁻³; 4.92 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):
7.80 × 10⁻⁸, 5.6 × 10⁻⁴, 2.1 × 10⁻⁴, 5.1 × 10⁻³, 8.0 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
1.58 × 10⁻⁵ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
6.026 × 10⁻⁶; 1.58 × 10⁻⁵ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
ln (P/Pa) = 38.743 – 16431/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (36.472 ± 0.679) – (15073 ± 282)/(T/K); temp range 403–428 K (Knudsen effusion technique, Li et al. 2004)
Henry’s Law Constant (Pa m³/mol):
1.096 (calculated-SOFA model, Govers & Krop 1998)
7.41; 1.096 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log K_{ow}:
6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
8.41 (calculated-QSAR, Fiedler & Schramm 1990)
7.36 (calculated-SOFA model, Govers & Krop 1998)
Chlorinated Dibenzo-\(p\)-dioxins

7.46; 7.36 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.20; 6.71, 6.78, 6.55, 6.87 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):
5.34 (calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, \( \log K_{OC} \):
5.91 (calculated-QSAR, Fiedler & Schramm 1990)
8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Volatilization:
Photolysis: \( t_\frac{1}{2} = 81.5 \) h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).
Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with \( NO_3 \) radical and \( k_{O_3} \) with \( O_3 \) as indicated, *data at other temperatures see reference:
\( k_{OH}(\text{calc}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Atkinson 1991)
\( k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) and a calculated tropospheric lifetime of 1.1 – 2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of 1.5 \( \times 10^6 \) molecule cm\(^{-3}\) at room temp. (Atkinson 1991)
\( k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated tropospheric lifetime of 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
\( k_1 = 61, 164 \) L kg\(^{-1}\) d\(^{-1}\); \( k_2 = 0.21, > 1.9 \) d\(^{-1}\) (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)
\( k_1 = 169 \) L kg\(^{-1}\) d\(^{-1}\), 251 L kg\(^{-1}\) d\(^{-1}\) (average \( k_1 \) for \( P_5\text{CDD} \) homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
Air: tropospheric lifetime \( \tau = 1.1–2.4 \) d calculated for a penta-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime \( \tau = 2.8–7.2 \) d for the gas-phase reaction with OH radical (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment: degradation \( t_\frac{1}{2} = 20–200 \) yr in sediment for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation \( t_\frac{1}{2} = 10–100 \) yr in soil (estimated, Suzuki et al. 2000).
Biota: half-lives in gold fish: \( t_\frac{1}{2} = 3.3 \) d for PBO treated and \( t_\frac{1}{2} > 1.9 \) d for control fish in 120-h exposure studies (Sijm et al. 1993).
8.1.1.20 1,2,3,4,7,8-Hexachlorodibenzo-\(p\)-dioxin

![Chemical Structure](image)

Common Name: 1,2,3,4,7,8-Hexachlorodibenzo-\(p\)-dioxin
Synonym: 1,2,3,4,7,8-H\(_6\)CDD
Chemical Name: 1,2,3,4,7,8-hexachlorodibenzo-\(p\)-dioxin
CAS Registry No: 39227–26–8
Molecular Formula: Cl\(_2\)C\(_6\)H\(_2\)O\(_2\)C\(_6\)Cl\(_4\)
Molecular Weight: 390.861

Melting Point (°C):
273–275 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)

Density (g/cm\(^3\) at 20°C):

- 206.96 (calculated-liquid density, Govers et al. 1990)
- 302.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):

- 89.1 (Rordorf 1987)

Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):

- 140.782 (Rordorf 1987)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):

- 48.1 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
- 30.21 (Friesen & Webster 1990)

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):

- 88 (Rordorf 1987, 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, \(F\): 0.00369 (assuming \(\Delta S_{fus} = 56\) J/mol K and mp at 273°C)

- 0.00352 (calculated-assuming \(\Delta S_{fus} = 56\) J/mol K, Shiu et al. 1988)
- 0.000148 (calculated-\(\Delta S_{fus}\) and mp, Passivirta et al. 1999)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- \(4.40 \times 10^{-6}\) (20°C, \(^{14}\)C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
- \(5.70 \times 10^{-6}\) (20°C, \(^{14}\)C-labeled, generator column-HPLC/LSC, Webster et al. 1986b)
- \(4.89 \times 10^{-6}\) (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
- \(1.00 \times 10^{-8}\) (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- \(1.45 \times 10^{-6}\) (supercooled liquid \(P_L\); GC-RT correlation, Falconer & Bidleman 1994)
- \(1.36 \times 10^{-9}\, 1.87 \times 10^{-9}\) (solid \(P_S\), calculated from reported \(P_L\), Delle Site 1997)
- \(3.19 \times 10^{-6}\) (corrected supercooled liquid \(P_L\); Eitzer & Hites 1998)
- \(5.20 \times 10^{-5}\, 7.70 \times 10^{-9}\) (supercooled liquid \(P_L\); converted to solid \(P_S\) with fugacity ratio \(F\), Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

- \(5.10 \times 10^{-9}\) (20°C, \(^{14}\)C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)
- \(3.20 \times 10^{-7}\) (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
- \(3.96 \times 10^{-6}\) (supercooled liquid \(P_L\), GC-RT correlation, Eitzer & Hites 1988, 1991)
- \(5.43 \times 10^{-6}\) (supercooled liquid \(P_L\), GC-RT correlation, Eitzer & Hites 1989)
- \(1.00 \times 10^{-8}\) (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- \(1.45 \times 10^{-6}\) (supercooled liquid \(P_L\), GC-RT correlation, Falconer & Bidleman 1994)
- \(1.36 \times 10^{-9}\, 1.87 \times 10^{-9}\) (solid \(P_S\), calculated from reported \(P_L\), Delle Site 1997)
- \(3.19 \times 10^{-6}\) (corrected supercooled liquid \(P_L\); Eitzer & Hites 1998)
- \(5.20 \times 10^{-5}\, 7.70 \times 10^{-9}\) (supercooled liquid \(P_L\); converted to solid \(P_S\) with fugacity ratio \(F\), Passivirta et al. 1999)
log \( \frac{P_s}{P_a} \) = 12.97 – 6282/(T/K) (solid, Passivirta et al. 1999)
log \( \frac{P_s}{P_a} \) = 8.37 – 3769/(T/K) (supercooled liquid, Passivirta et al. 1999)
log \( \frac{P_s}{P_a} = 15.65106 – 7087.08/(T/K) \) (regression eq. from literature data, Shiu & Ma 2000)
3.72 × 10⁻⁵ (supercooled liquid \( P_s \), Harner et al. 2000)
8.91 × 10⁻⁷ (supercooled liquid \( P_s \); GC-RI correlation; Wang & Wong 2002)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
0.452 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
0.631; 1.45 (quoted lit., calculated-SOFA model, Govers & Krop 1998)
log \( \frac{H}{P_a} \) = 8.14 – 1254/(T/K) (Passivirta et al. 1999)
0.427; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
10.36, 10.39, 10.89; 10.22, 10.44, 10.89 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
10.44, 7.79 (HPLC-RT correlation, Burkhart & Kuehl 1986)
7.80 (selected, Shiu et al. 1988)
8.0 (calculated-QSAR, Fiedler & Schramm 1990)
7.30 (calculated, Broman et al. 1991)
9.53 (HPLC-RT correlation, Chessells et al. 1991)
9.13 (calculated-fragment const., Chessells et al. 1991)
10.22 (quoted, Hansch et al. 1995)
7.94 (calculated-SOFA model, Govers & Krop 1998)
7.90 (estimated-solubility \( S_i \) and regression eq. using lit. \( K_{OW} \) values, Passivirta et al. 1999)
7.628 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.80; 7.12, 7.25, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
11.50 (calculated-\( K_{OW}/K_{AW} \), Wania & Mackay 1996)
11.17 (calculated, Finizio et al. 1997)
11.11*; 10.88 (generator column-GC; calculated, Harner et al. 2000)
12.20 (7°C, GC-retention time correlation, Harner et al. 2000)
log \( K_{OA} = -6.20 + 5160/(T/K) \); temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
10.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log \( BCF \):
3.73, 4.00 (rainbow trout, fathead minnow, steady-state, wet weight, Muir et al. 1985)
4.00, 5.00 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
3.41, 3.76 (fathead minnow, quoted, Opperhuizen & Sijm 1990)
3.45, 3.23 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.45, 4.87 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
5.01; 4.65 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
5.01; 5.01; 5.14 (guppy, 21-d exposure, lipid wt basis: measured-\( C_{inh}/C_{w} \); calculated; rate constant ratio \( k_1/k_2 \) from non-linear regression analysis, Loonen et al. 1994b)
5.01; 5.07 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
5.90, 5.98 (fish muscle log \( BCF_L \), calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log \( K_{OC} \) at 25°C or as indicated:
5.41, 5.31, 5.13 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
6.02, 6.15, 5.95 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986)
6.32, 6.27, 6.15 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
5.02 (DOC, De Voogt et al. 1990)
7.10 (Baltic Sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

**Volutilization:**

Photolysis:

\[ k(\text{calc}) = 1.06 \times 10^{-6} \text{ s}^{-1} \quad \text{with} \quad t_\frac{1}{2} = 7.57 \text{ d in spring}, \quad k = 0.676 \times 10^{-6} \text{ s}^{-1} \quad \text{with} \quad t_\frac{1}{2} = 11.87 \text{ d in autumn}, \quad k = 0.37 \times 10^{-6} \text{ s}^{-1} \quad \text{with} \quad t_\frac{1}{2} = 21.57 \text{ d in winter} \]

The averaged $k = 0.252 \times 10^{-6} \text{ s}^{-1}$ over full year with $t_\frac{1}{2} = 31.85 \text{ d}$, under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile (4:6 v/v) solution (Choudhary & Webster 1985a,c, 1986).

\[ k = 7.86 \times 10^{-6} \text{ s}^{-1} \quad \text{in water-acetonitrile (2:3, v/v) under direct sunlight} \quad \text{(Choudhary & Webster 1985b)} \]

\[ k = 7.86 \times 10^{-6} \text{ s}^{-1} \quad \text{with} \quad t_\frac{1}{2} = 24.5 \text{ h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons:} \]

\[ k_\text{HOH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{at room temp.} \quad \text{(Atkinson 1991)} \]

\[ k_\text{OH} = (4.6 - 6) \times 10^{-12} \text{ cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{and a calculated tropospheric lifetime} \quad \tau = 1.5 - 3.4 \text{ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of} \quad 1.5 \times 10^6 \text{ molecule/cm}^3 \quad \text{for a hexa-chlorinated dioxin at room temp.} \quad \text{(Atkinson 1991)} \]

**Oxidation:**

Rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO3}}$ with NO3 radical and $k_{\text{O3}}$ with O3 or as indicated, *data at other temperatures see reference:*

\[ k_\text{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{at room temp.} \quad \text{(Atkinson 1991)} \]

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

\[ k_1 = 102 \text{ d}^{-1}; \quad k_2 = 0.046 \text{ d}^{-1} \quad \text{(rainbow trout, flow-through system, Muir et al. 1985)} \]

\[ k_1 = 112 \text{ d}^{-1}; \quad k_2 = 0.030 \text{ d}^{-1} \quad \text{(fathead minnow, Muir et al. 1985)} \]

\[ k_1 = 0.030 \text{ d}^{-1} \quad \text{(fathead minnow, Muir & Yarechewski 1988)} \]

\[ k_1 = 0.015 \text{ d}^{-1} \quad \text{(rainbow trout, Muir & Yarechewski 1988)} \]

\[ k_2 = 0.0066 \text{ d}^{-1} \quad \text{(fathead minnow, Muir & Yarechewski 1988)} \]

\[ k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}; \quad k_2 = 299 \text{ L kg}^{-1} \text{ d}^{-1} \quad \text{(average $k_1$ for H6CDD homolog group, goldfish after 120-h exposure: metabolite inhibitor PBO-treated, control fish, Sijm et al. 1993)} \]

\[ k_2 = 0.29, > 0.02 \text{ d}^{-1} \quad \text{(goldfish after 120-h exposure: metabolite inhibitor PBO-treated, control, Sijm et al. 1993)} \]

\[ k_1 = 868 \text{ L kg}^{-1} \text{ d}^{-1}; \quad k_2 = 0.065 \text{ d}^{-1} \quad \text{(guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)} \]

\[ k_2 = 0.0105 \text{ d}^{-1} \quad \text{with} \quad t_\frac{1}{2} = 29 \text{ d (blue mussels, 99-d exposure, Hektoen et al. 1994)} \]

**Half-Lives in the Environment:**

Air: estimated reaction rate constant, $k = 0.005 \text{ h}^{-1}$ (Paterson et al. 1990);

tropospheric lifetime $\tau = 1.5 - 3.4 \text{ d for a hexa-chlorinated dioxin reaction with the OH radicals using a 12-h average daytime OH radical concn of} \quad 1.5 \times 10^4 \text{ molecule/cm}^3 \quad \text{(Atkinson 1991)}$;

photodegradation $t_\frac{1}{2} = 140 \text{ h in a rotary photoreactor absorbed to clean silica gel by filtered} \lambda < 290 \text{ nm of light, (Koester & Hites 1992)}$;

suggested $t_\frac{1}{2} = 740 \text{ h at} \quad 7^\circ \text{C for Baltic Proper environment (Sinkkonen & Pasivirto 2000)}$;

Surface water: under conditions of variable sunlight intensity at 40°N latitude: $t_\frac{1}{2} = 7.57 \text{ d in spring}, \quad t_\frac{1}{2} = 6.27 \text{ d in summer,} \quad t_\frac{1}{2} = 11.87 \text{ d in fall}, \quad t_\frac{1}{2} = 21.57 \text{ d in winter, and} \quad t_\frac{1}{2} = 76.8 \text{ d averaged over full year} \quad \text{(Choudhary & Webster 1985a, 1986)}$;

photolysis $t_\frac{1}{2} = 24.5 \text{ h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at} \quad 40^\circ \text{N latitude:} \quad 7.6 \text{ d in spring,} \quad 6.3 \text{ d in summer,} \quad 12.0 \text{ d in fall and} \quad 22.0 \text{ d in winter} \quad \text{(Choudhary & Webster 1989)}$;

$\tau = 81 \text{ d in sunlit surface water and} \quad \tau = 2.5 \text{ d in surface water of actual pond (Friesen et al. 1990)}$;
estimated reaction rate constant, \( k = 0.002 \) h\(^{-1}\) (Paterson et al. 1990);
suggested \( t_{1/2} = 14800 \) h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:
Sediment: estimated reaction rate constant \( k = 4.0 \times 10^{-6} \) h\(^{-1}\) (Paterson et al. 1990);
degradation \( t_{1/2} = 20–200 \) yr in sediment for all homologues (estimated, Suzuki et al. 2000);
suggested \( t_{1/2} = 2400000 \) h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: estimated reaction rate constant \( k = 2.8 \times 10^{-6} \) h\(^{-1}\) (Paterson et al. 1990);
degradation \( t_{1/2} = 10–100 \) yr in soil for all homologues (estimated, Suzuki et al. 2000);
suggested \( t_{1/2} = 2400000 \) h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: \( t_{1/2} = 43 \) d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);
half-lives in gold fish: \( t_{1/2} = 2.4 \) d for PBO treated and \( t_{1/2} = 40 \) d for control fish in 120-h exposure studies (Sijm et al. 1993);
\( t_{1/2} = 29 \) d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

---

**TABLE 8.1.1.20.1**

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7,8-hexachlorodibenzo-\( p \)-dioxin at various temperatures

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( S/g \cdot m^{-3} )</td>
<td>( S/g \cdot m^{-3} )</td>
<td>( P/Pa )</td>
<td>( \log K_{OA} )</td>
</tr>
<tr>
<td>20</td>
<td>( 4.40 \times 10^{-6} )</td>
<td>( 7 )</td>
<td>( 1.21 \times 10^{-6} )</td>
<td>( 25 )</td>
</tr>
<tr>
<td>40</td>
<td>( 1.90 \times 10^{-5} )</td>
<td>( 11.5 )</td>
<td>( 4.89 \times 10^{-6} )</td>
<td>( 75 )</td>
</tr>
<tr>
<td></td>
<td>( 17 )</td>
<td>( 26 )</td>
<td>( 21 )</td>
<td>( 125 )</td>
</tr>
</tbody>
</table>

\( \Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 48.1 \)
\( \Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 140.78 \)
\( \Delta S_{\text{fus}}/(\text{J mol}^{-1} \cdot \text{K}^{-1}) = 88 \)

\( \Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 98.70 \)

---
FIGURE 8.1.1.20.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 1,2,3,4,7,8-hexachlorodibenzo-$p$-dioxin.
8.1.1.21 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin

![Chemical Structure](image)

Common Name: 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin  
Synonym: 1,2,3,6,7,8-H6CDD  
Chemical Name: 1,2,3,6,7,8-hexachlorodibenzo-p-dioxin  
CAS Registry No: 57653–85–7  
Molecular Formula: Cl₃C₆H₂O₂C₆HCl₃  
Molecular Weight: 390.861  
Melting Point (°C):  
285  
(Ref: Lide 2003)  
Boiling Point (°C):  
487.7  
(calculated, Rordorf 1987, 1989)  
Density (g/cm³ at 20°C):  
(calculated-liquid density, Govers et al. 1990)  
302.4  
(calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):  
88.1  
(Rordorf 1987)  
Enthalpy of Sublimation, ΔHₛₜₐ₇ (kJ/mol):  
139.975  
(Rordorf 1987)  
Enthalpy of Fusion, ΔHₖₜₜ (kJ/mol):  
48.1  
(Rordorf 1987)  
Entropy of Fusion, ΔSₖₜₜ (J/mol K):  
86  
(Rordorf 1987, 1989)  
Fugacity Ratio at 25°C, F: 0.00281 (assuming ΔSₖₜₜ = 56 J/mol K and mp at 185°C)  
0.000167  
(calculated, Passivirta et al. 1999)  
Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):  
8.75 × 10⁻⁴ (calculated-SOFA model, Govers & Krop 1998)  
log [Sₙ/(mol/L)] = 0.125 – 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)  
1.10 × 10⁻³, 8.75 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):  
4.80 × 10⁻⁹, 3.80 × 10⁻⁷, 1.60 × 10⁻⁵, 4.0 × 10⁻⁴, 6.9 × 10⁻³ (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a, b, 1987, 1989)  
3.31 × 10⁻⁶ (supercooled liquid P₁, calculated-SOFA model, Govers & Krop 1998)  
5.20 × 10⁻⁴; 8.69 × 10⁻⁹ (supercooled liquid P₁; converted to solid P₃ with fugacity ratio F, Passivirta et al. 1999)  
log (P₁/P₄) = 12.96 – 6363/(T/K) (solid, Passivirta et al. 1999)  
log (P₁/P₄) = 8.47 – 3751/(T/K) (supercooled liquid, Passivirta et al. 1999)  
8.51 × 10⁻⁷, 3.31 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
Henry’s Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):  
1.45  
(calculated-SOFA model, Govers & Krop 1998)  
log [H/(Pa m³/mol)] = 8.35 – 1236/(T/K) (Passivirta et al. 1999)  
0.417; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)  
Octanol/Water Partition Coefficient, log Kₒₜₜₜ:  
9.13  
(calculated-QSAR, Fiedler & Schramm 1990)  
7.80  
(calculated, Broman et al. 1991)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:

12.22  (7°C, GC-retention time correlation, Harner et al. 2000)
10.97  (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.41, 4.61  (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.94; 4.70  (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.94; 5.05; 5.24  (guppies, 21-d exposure, lipid wt basis: measured-$C_{fish}/C_W$; calculated; rate constant ratio $k_1/k_2$ from non-linear regression analysis, Loonen et al. 1994b)
5.98  (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.56  (fish muscle log BCFL calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, log $K_{OC}$:

6.69  (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.60  (Baltic Sea particulate field samples, concentration-distribution-GC/MS, Broman et al. 1991)
9.42  (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatileization:

Photolysis: solution photolysis $t_{\frac{1}{2}} = 379$ min in n-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{\frac{1}{2}} = 44100$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);
photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{\frac{1}{2}} = 17.3$ h for native congener and $t_{\frac{1}{2}} = 14.2$ h for $^{13}$C-labeled congener in tetradecane solution (Tysklind & Rappe 1991);

$76.2$ h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with $NO_3$ radical and $k_{O3}$ with $O_3$ or as indicated, *data at other temperatures see reference: $k_{OH}$(calc) = (4.6 - 5.4) $\times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5$–3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6$ molecule/cm$^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 432$ L kg$^{-1}$ d$^{-1}$ (goldfish after 120-h exposure, control fish, Sijm et al. 1993)

$58$ L kg$^{-1}$ d$^{-1}; 299$ L kg$^{-1}$ d$^{-1}$ (average $k_1$ for $H_6CDD$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.23, < 0.1$ d$^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 844$ L kg$^{-1}$ d$^{-1}; k_2 = 0.050$ d$^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0075$ d$^{-1}$ with $t_{\frac{1}{2}} = 60$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991);
\[ t_{1/2} = 740 \text{ h at } 7^\circ\text{C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \]

Surface water: \[ t_{1/2} = 14800 \text{ h at } 7^\circ\text{C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).} \]

Groundwater:

Sediment: degradation \[ t_{1/2} = 20–200 \text{ yr in sediment for all homologues (estimated, Suzuki et al. 2000);} \]

\[ t_{1/2} = 550000 \text{ h at } 7^\circ\text{C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).} \]

Soil: degradation \[ t_{1/2} = 10–100 \text{ yr in soil for all homologues (estimated, Suzuki et al. 2000);} \]

\[ t_{1/2} = 550 000 \text{ h at } 7^\circ\text{C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).} \]

Biota: 43 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

\[ t_{1/2} = 3.0 \text{ d for PBO treated gold fish, } t_{1/2} > 7 \text{ d for control fish in 120-h exposure studies (Sijm et al. 1993);} \]

\[ t_{1/2} = 40 \text{ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).} \]
8.1.1.22 1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin

Common Name: 1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin
Synonym: 1,2,3,7,8,9-H6CDD OR 2,3,4,6,7,8-H6CDD
Chemical Name: 1,2,3,7,8,9-hexachlorodibenzo-p-dioxin
CAS Registry No: 19408–74–3
Molecular Formula: Cl3C6HO2C6HCl3
Molecular Weight: 390.861
Melting Point (°C):
  243–244 (Rordorf 1987)
Boiling Point (°C):
  487.7 (calculated, Rordorf 1987, 1989)
Density (g/cm³ at 20°C):
  207.16 (calculated-liquid density, Govers et al. 1990)
  210.16 (liquid molar volume, Govers et al. 1995)
  301.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
  91.7 (Rordorf 1987)
  103.9 (GC-RI correlation, Govers et al. 1995)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
  142.922 (Rordorf 1987)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
  48.1 (Rordorf 1987)
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
  93 (Rordorf 1987, 1989)
Fugacity Ratio at 25°C, F:
  0.00027 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):
  6.34 × 10⁻⁴ (calculated-SOFA model, Govers & Krop 1998)
  \[ \log [S_s/(mol/L)] = 0.491 - 2515/(T/K) \] (liquid, Passivirta et al. 1999)
  1.10 × 10⁻³, 6.34 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
  6.50 × 10⁻⁹, 5.60 × 10⁻⁷, 2.60 × 10⁻⁵, 7.00 × 10⁻⁴, 1.30 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
  1.38 × 10⁻⁶ (calculated-SOFA model, Govers & Krop 1998)
  4.51 × 10⁻³; 1.22 × 10⁻³ (supercooled liquid \( P_s \); converted to solid \( P_s \) with fugacity ratio F, Passivirta et al. 1999)
  \[ \log (P_s/Pa) = 12.93 - 6211/(T/K) \] (solid, Passivirta et al. 1999)
  \[ \log (P_s/Pa) = 8.07 - 3699/(T/K) \] (supercooled liquid, Passivirta et al. 1999)
  8.51 × 10⁻⁷, 1.38 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Henry’s Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):
  0.832 (calculated-SOFA model, Govers & Krop 1998)
  \[ \log [H/(Pa m³/mol)] = 7.58 - 1184/(T/K) \] (Passivirta et al. 1999)
  0.417; 0.832 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, \( \log K_{ow} \):
  6.90 (calculated, Broman et al. 1991)
Chlorinated Dibenzo-\(p\)-dioxins

8.02 (calculated-SOFA model, Govers & Krop 1998)
7.76 (estimated-solubility \(S_L\) and regression eq. using lit. \(K_{OW}\) values, Passivirta et al. 1999)
7.61 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.95; 8.02 (GC-R1 correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log \(K_{OA}\) at 25°C or as indicated:
12.26 (7°C, GC-retention time correlation, Harner et al. 2000)
11.01 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log \(BCF\):
2.95 (guppy exposed to fly ash extract, Opperhuizen et al. 1986)
3.50, 4.02 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.93; 4.34 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-\(C_{fish}/C_{W}\); calculated; rate constant ratio \(k_1/k_2\) from nonlinear regression analysis, Loonen et al. 1994b)
5.18 (calculated-SOFA model, Govers & Krop 1998)
5.29 (fish muscle log \(BCF_L\) calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, log \(K_{OC}\):
6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
6.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
9.45 (calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):

Volatilization:
Photolysis: photolytic \(t_{1/2} = 5.4\) h when exposed to sunlight in hexane solution (Doobs & Grant 1979)
photolytic degradation \(t_{1/2} = 17.1\) h in extract from fly ash exposed to UV light from a distance of 20 cm in tetradecane solution (Tysklind & Rappe 1991)
\(t_{1/2} = 92.4\) h on spruce needle surface under sunlight irradiation (Niu et al. 2003).
Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO_3}\) with NO\(_3\) radical and \(k_{O_3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:
\(k\) (oxidative degradation rate constant of water dissolved PCDD) is \(5.02 \times 10^4\) L g\(^{-1}\) min\(^{-1}\) under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)
\(k_{OH(calc)} = (4.6 – 5.4) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at room temp. (Atkinson 1991)
\(k_{OH} = (4.6 – 10) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) and a calculated tropospheric lifetime of 1.5 – 3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of \(1.5 \times 10^6\) molecule cm\(^{-3}\) for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \(k_1\) and Elimination \(k_2\) Rate Constants:
\(k_1 = 200\) mL g\(^{-1}\) d\(^{-1}\); \(k_2 = 0.210\) d\(^{-1}\) (guppy, Opperhuizen et al. 1986)
\(k_1 = 48, 433\) L kg\(^{-1}\) d\(^{-1}\); \(k_2 = 0.44, < 0.1\) d\(^{-1}\) (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)
\(k_1 = 58\) L kg\(^{-1}\) d\(^{-1}\), 299 L kg\(^{-1}\) d\(^{-1}\) (average \(k_1\) for H\(_6\)CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
\(k_1 = 687\) L kg\(^{-1}\) d\(^{-1}\); \(k_2 = 0.074\) d\(^{-1}\) (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)
\(k_2 = 0.0057\) d\(^{-1}\) with \(t_{1/2} = 52\) d (blue mussel, 99-d exposure, Hektoen et al. 1994)
Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

$\tau_{1/2} = 740$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $\tau_{1/2} = 14800$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $\tau_{1/2} = 20$–200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

$\tau_{1/2} = 2400000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $\tau_{1/2} = 10$–100 yr in soil for all homologues (estimated, Suzuki et al. 2000);

$\tau_{1/2} = 2400000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: half-lives in gold fish: 1.6 d for PBO treated and $\tau_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$\tau_{1/2} = 52$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).
8.1.1.23 1,2,4,6,7,9-Hexachlorodibenzo-p-dioxin

Common Name: 1,2,4,6,7,9-Hexachlorodibenzo-p-dioxin
Synonym: 1,2,4,6,7,9-H6CDD
Chemical Name: 1,2,4,6,7,9-hexachlorodibenzo-p-dioxin
CAS Registry No: 39227–62–8
Molecular Formula: Cl₆C₆H₂O₂Cl₃
Molecular Weight: 390.861

Melting Point (°C):
238–240 (Pohland & Yang 1972, Rordorf 1987)

Boiling Point (°C):
487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):
215.5 (calculated-liquid density, Govers et al. 1990)
302.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHV (kJ/mol):
92.1 (Rordorf 1987)

Enthalpy of Sublimation, ΔHsubl (kJ/mol):
143.238 (Rordorf 1987)

Enthalpy of Fusion, ΔHfus (kJ/mol):
48.1 (Rordorf 1987)

Entropy of Fusion, ΔSfus (J/mol K):
94 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):
0.00187 (calculated-SOFA model, Govers & Krop 1998)
1.71 × 10⁻³, 1.87 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
6.80 × 10⁻⁹, 5.9 × 10⁻⁷, 2.7 × 10⁻⁵, 7.5 × 10⁻⁴, 1.40 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
1.41 × 10⁻⁶ (supercooled liquid Pt, calculated-SOFA model, Govers & Krop 1998)
1.35 × 10⁻⁶, 1.41 × 10⁻⁵ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry’s Law Constant (Pa m³/mol at 25°C):
0.0282 (calculated-SOFA model, Govers & Krop 1998)
0.479; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log Kow:
7.85 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989a)
7.73 (calculated-SOFA model, Govers & Krop 1998)
7.84; 7.73 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
6.85; 7.05, 7.26, 6.96, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF:
5.36 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log $K_{OC}$:
8.99 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\text{1/2}$:

Volatilization:
Photolysis: photolytic $t_\text{1/2} = 47$ h when exposed to sunlight in hexane solution (Doobs & Grant 1979); solution
photolysis $t_\text{1/2} = 764$ min in n-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis
$c_\text{1/2} = 7870$ min on a clean glass surface under the same conditions (Nestrick et al. 1980)

Hydrolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$
with NO$_3$ radical and $k_{O3}$ with O$_3$ as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5-3.4$ d based on
gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6$ molecule/cm$^3$
for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 88, 82$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.62, > 0.8$ d$^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure
studies, Sijm et al. 1993)

$k_1 = 58$ L kg$^{-1}$ d$^{-1}$, 299 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for H$_6$CDD homolog group, goldfish after 120-h exposure:
metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$, the tropospheric lifetime of a
hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical
(Atkinson 1991)

Surface water:
Groundwater:
Sediment: degradation $t_\text{1/2} = 20–100$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).
Soil: degradation $t_\text{1/2} = 10–100$ yr in soil or all homologues (estimated, Suzuki et al. 2000).
Biota: half-lives in gold fish: $t_\text{1/2} = 1.1$ d for PBO treated and $t_\text{1/2} < 0.9$ d for control fish in 120-h exposure studies
(Sijm et al. 1993).
8.1.1.24 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin

Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin
Synonym: 1,2,3,4,6,7,8-H$_7$CDD
Chemical Name: 1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin
CAS Registry No: 35822–46–9
Molecular Formula: Cl$_3$C$_6$HO$_2$C$_6$Cl$_4$
Molecular Weight: 425.308

Melting Point (°C):
264–265  (Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):
507.2  (Rordorf 1987,1989)

Density (g/cm$^3$ at 20°C):
Molar Volume (cm$^3$/mol):
218.32  (calculated-liquid density, Govers et al. 1990)
323.3  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta$H$_v$ (kJ/mol):
92.5  (Rordorf 1987)

Enthalpy of Sublimation, $\Delta$H$_{subl}$ (kJ/mol):
149.792  (Rordorf 1987)

Enthalpy of Fusion, $\Delta$H$_{fus}$ (kJ/mol):
53.9  (Rordorf 1987; quoted, Ruelle & Kesselring 1997)
30.42  (Friesen & Webster 1990)

Entropy of Fusion, $\Delta$S$_{fus}$ (J/mol K):
100  (Rordorf 1987,1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.00442 (assuming $\Delta$S$_{fus}$ = 56 J/mol K and mp at 265°C)
0.00423  (calculated-assuming $\Delta$S$_{fus}$ = 56 J/mol K, Shiu et al. 1988)
6.11 × 10$^{-5}$  (calculated-$\Delta$S$_{fus}$ and mp, Passivirta et al. 1999)

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.40 × 10$^{-9}$, 2.42 × 10$^{-9}$  (20°C, 14C-labeled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)
2.30 × 10$^{-6}$*  (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)
log [S$_L$/(mol/L)] = 0.391 – 2820/(T/K) (supercooled liquid, Passivirta et al. 1999)
3.15 × 10$^{-4}$  (supercooled liquid S$_L$, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.20 × 10$^{-8}$  (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)
1.02 × 10$^{-6}$  (supercooled liquid P$_L$, GC-RT correlation, Eitzer & Hites 1988, 1991)
1.19 × 10$^{-6}$  (supercooled liquid, GC/MS, Eitzer & Hites 1989)
3.20 × 10$^{-9}$  (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
4.41 × 10$^{-9}$, 5.15 × 10$^{-9}$  (solid P$_S$, calculated from reported P$_L$, Delle Site 1997)
8.97 × 10$^{-6}$  (corrected supercooled liquid P$_L$, Eitzer & Hites 1998)
6.03 × 10$^{-2}$, 5.89 × 10$^{-2}$  (supercooled liquid P$_L$, quoted expltl., calculated-SOFA model, Govers & Krop 1998)
8.97 × 10$^{-6}$, 6.79 × 10$^{-10}$  (supercooled liquid P$_L$; converted to solid P$_S$ with fugacity ratio F, Passivirta et al. 1999)
log (P_s/P_a) = 13.18 – 6661/(T/K) (solid, Passivirta et al. 1999)
log (P_l/P_a) = 7.95 – 3844/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P/P_a) = 17.10357 – 7820.06/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
2.04 x 10⁻⁷, 5.89 x 10⁻⁷ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry’s Law Constant (Pa m²/mol at 25°C and the reported temperature dependence equations):
0.133 (calculated-P/C, Shiu et al. 1988)
4.25 (computed-expert system SPARC, Kollig 1995)
0.832 (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m²/mol)] = 7.56 – 7024/(T/K) (Passivirta et al. 1999)
0.275; 0.832 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:
11.29, 11.42, 11.90; 11.03, 11.50, 11.98 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
11.05, 11.50 (HPLC-RT correlation, Sarna et al. 1984)
11.38, 10.55; 11.05, 9.69 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
8.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)
11.03 (Hansch et al. 1995)
8.85 (computed-expert system SPARC, Kollig 1995)
8.40 (calculated-SOFA model, Govers & Krop 1998)
8.31 (estimated-solubility S_w and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)
8.051 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.27; 8.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
7.66, 7.43, 8.18, 7.73 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
11.42*; 10.73 (generator column-GC, measured range 20–50°C, calculated, Harner et al. 2000)
log K_{oa} = –3.51 + 4450/(T/K); temp range 30–50°C (Harner et al. 2000)

Bioconcentration Factor, log BCF:
3.32, 3.74 (fathead minnow, rainbow trout, steady-state, wet weight, Muir et al. 1985)
3.32, 4.32 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
2.92, 4.28 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
4.68 (guppy, Loonen et al. 1994)
4.68; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.68; 4.68; 4.76 (guppies, 21-d exposure, lipid wt basis: measured-C_{fish}/C_{w}; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.68; 4.79 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
6.11, 6.34 (fish muscle log BCF_{L} calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{oc}:
6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
5.47 (DOC, De Voogt et al. 1990)
7.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
10.95; 10.0 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, t_½:
Volatilization:
Photolysis:
photolytic t_½ = 11 h in n-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
solution photolysis t_½ = 1800 min at 1.0 m from a GE Model sunlamp and surface photolysis t_½ = 3140 min on clean soft glass surface under the same conditions (Nestrick et al. 1980)
t_{1/2} = 30 \text{ h in } n\text{-hexadecane solution (Mamantov 1984)};

first order k = 1.02 \times 10^{-6} \text{ s}^{-1} in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: t_{1/2} = 56.46 \text{ d in spring}; t_{1/2} = 47.33 \text{ d in summer}; t_{1/2} = 87.86 \text{ d in autumn}; t_{1/2} = 155.79 \text{ d in winter and averaged } t_{1/2} = 2993 \text{ d over full year (Choudhary & Webster 1985b, 1986)}.

photolysis k = 1.02 \times 10^{-6} \text{ s}^{-1} with t_{1/2} = 191 \text{ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: } k = 1.24 \times 10^{-2} \text{ d}^{-1} \text{ with } t_{1/2} = 57 \text{ d in spring}; k = 1.48 \times 10^{-2} \text{ d}^{-1} \text{ with } t_{1/2} = 47 \text{ d in summer}; k = 0.80 \times 10^{-2} \text{ d}^{-1} \text{ with } t_{1/2} = 88 \text{ d in autumn}; k = 0.45 \times 10^{-2} \text{ d}^{-1} \text{ with } t_{1/2} = 156 \text{ d in winter (Choudhary & Webster 1989)}.

sunlight photolysis k = 0.28 \text{ d}^{-1} in filtered and sterilized natural water and k = 0.019 \text{ d}^{-1} in (2:32, v/v) distilled water-acetonitrile solution at 50°N (Friesen et al. 1990).

photolytic t_{1/2} = 53.4 \text{ h for native congener and } t_{1/2} = 32.6 \text{ h in } ^{13}C\text{-labeled congener in extract from fly ash (Tysklind & Rappe 1991).}

tropospheric lifetime was calculated based on the gas-phase reaction rate constant k = (4.6-10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} with the OH radicals to be 1.5-2.4 \text{ d (Atkinson 1991)}.

photodegradation rate constant k = 0.18 \text{ h}^{-1} \text{ with } t_{1/2} = 3.9 \text{ h when loaded on TiO}_2 \text{ film under UV (} \lambda > 300 \text{ nm) or solar light irradiation in the air (Choi et al. 2000)}.

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD by ozone) = 5.46 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1} under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987).

k_{OH}\text{(calc)} = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} and a calculated tropospheric lifetime } \tau = 4.4 \text{ d based on gas phase OH reactions and a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule/cm}^3 \text{ for a hepta-chlorinated dioxin at room temp. (Atkinson 1991)}.

Hydrolysis:

Biodegradation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 56 \text{ d}^{-1}; k_2 = 0.042 \text{ d}^{-1} (rainbow trout exposed to concn of 11, 55 pg/L, Muir et al. 1985).

k_1 = 19 \text{ d}^{-1}; k_2 = 0.040 \text{ d}^{-1} (fathead minnow exposed to concn of 8, 39 pg/L, Muir et al. 1985).

k_1 = 0.048 \text{ d}^{-1} (fathead minnow, Muir & Yarechewski 1988).

k_1 = 0.0092 \text{ d}^{-1} (fathead minnow, quoted, Oppenhuizen & Sijm 1990).

k_1 = 0.0110 \text{ d}^{-1} (rainbow trout, quoted, Oppenhuizen & Sijm 1990).

k_1 = 32, 150 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.49, > 0.12 \text{ d}^{-1} (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993).

k_1 = 23 \text{ L kg}^{-1} \text{ d}^{-1}, 167 \text{ L kg}^{-1} \text{ d}^{-1} (average } k_1 \text{ for } P_2\text{CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993).

k_1 = 456 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.081 \text{ d}^{-1} (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b).

k_2 = 0.0061 \text{ d}^{-1} with } t_{1/2} = 49 \text{ d (blue mussel, 99-d exposure, Hektoen et al. 1994)}.

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 \times 10^6 \text{ molecule cm}^{-3}, the tropospheric lifetime } \tau = 4.4 \text{ d for a hepta-PCDD for the gas-phase reaction with OH radicals (Atkinson 1991)};

suggested } t_{1/2} = 1500 \text{ h at } 7°C \text{ for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000)};

first-order photodegradation k = 0.19 \text{ h}^{-1} \text{ with } t_{1/2} = 3.9 \text{ h when loaded on TiO}_2 \text{ film under UV (} \lambda > 300 \text{ nm) or solar light irradiation in the air (Choi et al. 2000)}.

Surface water: } t_{1/2} = 11 \text{ h in } n\text{-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)};

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: } t_{1/2} = 56.46 \text{ d in spring}; t_{1/2} = 47.33 \text{ d in summer}; t_{1/2} = 87.86 \text{ d in autumn}; t_{1/2} = 155.79 \text{ d in winter and averaged } t_{1/2} = 2393 \text{ d over full year (Choudhary & Webster 1985b, 1986)};
photolysis $t_{1/2} = 190.97$ h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season
direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 57$ d in spring, $t_{1/2} = 47$ d
in summer, $t_{1/2} = 88$ d in fall and $t_{1/2} = 156$ d in winter (Choudhary & Webster 1989);
$t_{1/2} = 81$ d in sunlit filtered and sterilized surface water and $t_{1/2} = 2.5$ d in surface water of actual pond at
50°N latitude (Friesen et al. 1990);
$t_{1/2} = 53.4$ and $32.6$ h in native and $^{13}$C-labeled congeners, respectively, in extract from fly ash (Tysklind &
Rappe 1991);
suggested $t_{1/2} = 30000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:
Sediment: degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000);
suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).
Soil: degradation $t_{1/2} = 10–100$ yr in soil (estimated, Suzuki et al. 2000);
suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).
Biota: $t_{1/2} = 17.2$ d in fathead minnow (Adams et al. 1986);
$t_{1/2} > 336$ d in carp (Kuehl et al. 1987);
$t_{1/2} = 39$ d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);
$t_{1/2} = 27.2$ d in lactating cows (Olling et al. 1991);
half-lives in gold fish: $t_{1/2} = 1.4$ d for PBO treated and $t_{1/2} = 5.6$ d for control fish in 120-h exposure studies
(Sijm et al. 1993);
$t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

### TABLE 8.1.1.24.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,6,7,8-
heptachlorodibenzo-p-dioxin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-HPLC/LSC</td>
<td>generator column-HPLC/LSC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>20</td>
<td>$2.40 \times 10^{-6}$</td>
<td>7</td>
</tr>
<tr>
<td>40</td>
<td>$6.30 \times 10^{-5}$</td>
<td>11</td>
</tr>
<tr>
<td>17</td>
<td>$1.29 \times 10^{-6}$</td>
<td>75</td>
</tr>
<tr>
<td>21</td>
<td>$2.30 \times 10^{-6}$</td>
<td>100</td>
</tr>
<tr>
<td>26</td>
<td>$2.56 \times 10^{-6}$</td>
<td>125</td>
</tr>
<tr>
<td>41</td>
<td>$6.34 \times 10^{-5}$</td>
<td></td>
</tr>
</tbody>
</table>

$\Delta H_{fluid}/(kJ \cdot mol^{-1}) = 92.5$
$\Delta H_{subl}/(kJ \cdot mol^{-1}) = 149.79$
$\Delta H_{fus}/(kJ \cdot mol^{-1}) = 53.9$
$\Delta S_{fus}/(J \cdot mol^{-1} \cdot K^{-1}) = 100$
$\Delta H_{OA}/(kJ \cdot mol^{-1}) = 85.10$
FIGURE 8.1.1.24.1 Logarithm of mole fraction solubility, vapor pressure and $K_{OA}$ versus reciprocal temperature for 1,2,3,4,6,7,8-heptachlorodibenzo-$p$-dioxin.
8.1.1.25 1,2,3,4,7,8,9-Heptachlorodibenzo-\(p\)-dioxin

Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzo-\(p\)-dioxin
Synonym: 1,2,3,4,7,8,9-H\(_7\)CDD
Chemical Name: 1,2,3,4,7,8,9-heptachlorodibenzo-\(p\)-dioxin
CAS Registry No:
Molecular Formula: Cl\(_3\)C\(_6\)HO\(_2\)C\(_6\)Cl\(_4\)
Molecular Weight: 425.308
Melting Point (°C):
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
Molar Volume (cm\(^3\)/mol):
  222.55 (calculated-liquid density, Govers et al. 1990)
  323.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
Enthalpy of Sublimation, \(\Delta H_{sub}\) (kJ/mol):
Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
Fugacity Ratio at 25°C, \(F\):
Water Solubility (g/m\(^3\) or mg/L at 25°C):
  4.57 \times 10^{-4} (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)
  3.97 \times 10^{-4}, 4.57 \times 10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C):
  3.39 \times 10^{-7} (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)
  2.57 \times 10^{-7}, 3.39 \times 10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Henry’s Law Constant (Pa m\(^3\)/mol):
  0.309 (calculated-SOFA model, Govers & Krop 1998)
  0.295; 0.309 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log \(K_{OW}\):
  8.25 (calculated-SOFA model, Govers & Krop 1998)
  8.22; 8.25 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Air Partition Coefficient, log \(K_{OA}\):
Bioconcentration Factor, log \(BCF\):
  4.95 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
Sorption Partition Coefficient, log \(K_{OC}\):
  9.75 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{0.5}\):
  Volatilization:
    Photolysis: photolytic \(t_{0.5} = 27\) h when exposed to sunlight in hexane solution (Dobbs & Grant 1979)
    Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\)
      with NO\(_3\) radical and \(k_{O3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:
Chlorinated Dibenzo-\(p\)-dioxins

\( k \) (oxidative degradation rate constant of water dissolved PCDD by ozone) is \( 5.46 \times 10^4 \) \( \text{L g}^{-1} \text{min}^{-1} \) under alkaline condition at \( \text{pH} \) 10 and 20\(^\circ\)C (Palaschek & Scholz 1987)

\( k_{\text{OH(calc)}} = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) and a calculated tropospheric lifetime \( \tau = 4.4 \) d based on gas phase OH reactions and a 12-h average daytime OH radical concn of \( 1.5 \times 10^6 \) molecule/cm\(^3\) for a hepta-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[ k_1 = 12 \text{ L kg}^{-1} \text{ d}^{-1}, \quad 183 \text{ L kg}^{-1} \text{ d}^{-1}; \quad k_2 = 1.3 \text{ d}^{-1}, \quad >3.4 \text{ d}^{-1} \] (metabolic inhibitor PBO-treated goldfish, control goldfish, 120-h exposure studies, Sijm et al. 1993)

\[ k_1 = 22 \text{ L kg}^{-1} \text{ d}^{-1}, \quad 167 \text{ L kg}^{-1} \text{ d}^{-1} \] (average \( k_1 \) for \( \text{H}_7\text{CDD} \) homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of \( 1.5 \times 10^6 \) molecule/cm\(^3\), the tropospheric lifetime of a hepta-PCDD was calculated to be 4.4 d for the gas-phase reaction with OH radical (Atkinson 1991)

Surface water:

Groundwater:

Sediment: degradation \( t_{1/2} = 20-200 \) yr in sediment for all homologues (estimated, Suzuki et al. 2000)

Soil: degradation \( t_{1/2} = 10-100 \) yr in soil (estimated, Suzuki et al. 2000)

Biota: half-lives in gold fish: \( t_{1/2} = 0.5 \text{ d} \) for PBO treated and \( t_{1/2} <0.2 \text{ d} \) for control fish in 120-h exposure studies (Sijm et al. 1993).
8.1.1.26 Octachlorodibenzo-\(p\)-dioxin

\[
\begin{array}{c}
\text{Cl} \quad \text{O} \\
\text{C}_{12}\text{Cl}_8\text{O}_2 \\
\text{Cl}_4\text{C}_6\text{O}_2\text{C}_6\text{Cl}_4
\end{array}
\]

Common Name: Octachlorodibenzo-\(p\)-dioxin

Synonym: O\(8\)CDD, OCDD

Chemical Name: octachlorodibenzo-\(p\)-dioxin

CAS Registry No: 3268–87–9

Molecular Formula: \(\text{C}_{12}\text{Cl}_8\text{O}_2\), \(\text{Cl}_4\text{C}_6\text{O}_2\text{C}_6\text{Cl}_4\)

Molecular Weight: 459.751

Melting Point (\(^\circ\)C):

331 (Lide 2003)

Boiling Point (\(^\circ\)C):

510 (Rordorf 1987, 1989)

Density (g/cm\(^3\) at 20\(^\circ\)C):

Molar Volume (cm\(^3\)/mol):

- 229.6, 229.11 (calculated-liquid density, crystalline volume, Govers et al. 1990)
- 237.21 (liquid molar volume, Govers et al. 1995)
- 344.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):

86.7 (Rordorf 1987)

Enthalpy of Sublimation, \(\Delta H_{\text{subl}}\) (kJ/mol):

151.13 (Rordorf 1987)
145.7 (Li et al. 2004)

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):

61.4 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):

102 (Rordorf 1986, 1987, 1989; Passivirta et al. 1999)

Fugacity Ratio at 25\(^\circ\)C, \(F\): 0.000995 (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K and mp at 331\(^\circ\)C)

- 0.00107 (calculated-assuming \(\Delta S_{\text{fus}} = 56\) J/mol K, Shiu et al. 1987)
- 0.00115 (calculated-assuming \(\Delta S_{\text{fus}} = 56\) J/mol K, Shiu et al. 1988)
- 3.46 \times 10^{-6} (calculated-\(\Delta S_{\text{fus}}\) and mp, Passivirta et al. 1999)

Water Solubility (g/m\(^3\) or mg/L at 25\(^\circ\)C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2.0 \times 10^{-6} (Barrie et al. 1983)
- 4.0 \times 10^{-7} (\(^{14}\)C-labeled, generator column-HPLC/LSC, Webster et al. 1983)
- 4.0 \times 10^{-7} (20\(^\circ\)C, \(^{14}\)C-labeled, generator column-HPLC/LSC, measured range 20–40\(^\circ\)C, Friesen et al. 1985)
- 4.0 \times 10^{-7} (20\(^\circ\)C, \(^{14}\)C-labeled, generator column-HPLC/LSC, measured range 20–40\(^\circ\)C, Webster et al. 1985)
- 1.8 \times 10^{-4} (Opperhuizen 1986)
- 1.0 \times 10^{-7} (\(^{14}\)C-labeled-LSC, Srinivasan & Fogler 1987)
- 7.4 \times 10^{-8} (extrapolated, generator column-GC/ECD, measured range 40–80\(^\circ\)C, Doucette & Andren 1988a)

\(S/(\text{mol}/\text{L}) = 8.32 \times 10^{-6} \exp(0.041\cdot t/\text{°C})\) (generator column-GC/ECD, temp range 40–80\(^\circ\)C, Doucette & Andren 1988a)

\[
\log x = -3891/(T/K) - 1.482; \text{ temp range 40–80°C (generator column-GC/ECD, Doucette & Andren 1988a)}
\]

\[
\log [S_L/(\text{mol}/\text{L})] = -0.163 - 3212/(T/K) \text{ (supercooled liquid, Passivirta et al. 1999)}
\]

1.03 \times 10^{-4} (supercooled liquid \(S_L\), GC-RI correlation; Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.40 × 10⁻⁵, 1.8 × 10⁻⁵ (quoted, calculated-volatilization rate, Dobbs & Cull 1982)
8.70 × 10⁻⁶ (20°C, gas saturation, Webster et al. 1985)
1.10 × 10⁻¹⁰* (gas saturation, Rordorf 1985a,b, 1986a,b, 1987, 1989)
2.51 × 10⁻¹⁰ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf 1986)
2.74 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988)
2.77 × 10⁻⁷ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1991)
2.72 × 10⁻⁷ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
0.000280* (120.1°C, average value, gas saturation-GC, measured range 120.1–199.7°C, Rordorf 1990)
1.60 × 10⁻¹⁰ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substituted no. plot, Rordorf et al. 1990)
2.62 × 10⁻¹⁰, 2.56 × 10⁻¹⁰ (solid P_S, calculated from reported P_L, Delle Site 1997)
2.75 × 10⁻⁹ (correcting supercooled liquid P_L value of 1988, Eitzer & Hites. 1998)
1.82 × 10⁻⁷; 1.35 × 10⁻⁷ (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
2.75 × 10⁻⁷; 4.92 × 10⁻¹² (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P/Pa) = 15.81886 − 7629.38/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0912* (175°C, Knudsen effusion method, measured range, 175–220°C, Li et al. 2002)
log (P/Pa) = 13.62 − 7429/(T/K) (solid, Passivirta et al. 1999)
log (P/Pa) = 8.32 − 4221/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln (P/Pa) = (32.825 ± 0.153) − (15773 ± 72)/(T/K); temp range 448–493 K (Knudsen effusion method, Li et al. 2002)
log (P/Pa) = 38.156 − 16431/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (36.461 ± 1.020) − (17529 ± 487)/(T/K); temp range 463–493 K (Knudsen effusion technique, Li et al. 2004)

Henry’s Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

0.683 (calculated-P/C, Shiu et al. 1987,1988)
1.32; 0.513 (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m³/mol)] = 8.34 − 1009/(T/K) (Passivirta et al. 1999)
0.191; 0.513 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_OW:

8.50 (Bruggeman et al. 1984; quoted, Opperhuizen 1986)
12.21, 12.60, 12.97; 11.82, 12.72, 13.08 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
11.16, 12.72 (HPLC-RT correlation, Sarna et al. 1984)
10.56, 7.53 (calculated-TSA, Doucette 1985)
12.26, 11.35; 11.76, 10.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
8.60 (HPLC-RT correlation, Burkhard & Kuehl 1986)
7.59 (generator column-GC/ECD, Doucette & Andren 1987)
7.83 (HPLC-RT correlation, Doucette and Andren 1988b)
8.60 (calculated, Endicott & Cook 1994)
7.59, 8.60 (quoted, Hansch et al. 1995)
9.31 (estimated-solubility S_i and regression eq. using lit. K_OW values, Passivirta et al. 1999)
8.450 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.48 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_OA at 25°C or as indicated:

10.80 (calculated-K_OW/K_AW, Wania & Mackay 1996)
13.0 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:

1.93, 3.35 (fathead minnow; rainbow trout, steady-state, wet weight, Muir et al. 1985,1986)
1.53–2.13; 3.35 (fathead minnow, rainbow trout, Muir et al. 1986)
<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00, 2.05</td>
<td>(human fat, calculated-lipid base, Geyer et al. 1987)</td>
<td></td>
</tr>
<tr>
<td>0.903, 1.93</td>
<td>(human fat, calculated-wet wt. base, Geyer et al. 1987)</td>
<td></td>
</tr>
<tr>
<td>1.90, 3.10</td>
<td>(guppy: in whole fish, in lipid, Gobas et al. 1987)</td>
<td></td>
</tr>
<tr>
<td>6.33, 5.85</td>
<td>(plant parts, calculated-vapor pressure; calculated-vapor pressure &amp; HLC, Reischl et al. 1989)</td>
<td></td>
</tr>
<tr>
<td>2.85, 3.97</td>
<td>(guppy: wet weight base, lipid weight base, Gobas &amp; Schrap 1990; quoted, Devillers et al. 1996)</td>
<td></td>
</tr>
<tr>
<td>2.85</td>
<td>(predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.25, 2.32</td>
<td>(ganged invertebrates exposed to water concn. 2.0 ng/L for 0–10 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.32</td>
<td>(caged unionid clams exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.42, 2.34</td>
<td>(caged invertebrates exposed to water concn. 0.6 ng/L for 14–24 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>1.89</td>
<td>(predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.75</td>
<td>(caged white suckers gill exposed to water concn. 1.3 ng/L for 14–24 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.24, 3.97</td>
<td>(caged white suckers carcass exposed to water concn. 2.8 ng/L for 0–104 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.24</td>
<td>(caged white suckers carcass exposed to water concn. 0.4 ng/L for 14–24 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>2.75</td>
<td>(caged white suckers gill exposed to water concn. 1.3 ng/L for 14–24 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>1.89</td>
<td>(predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>3.97</td>
<td>(caged white suckers carcass exposed to water concn. 2.7 ng/L for 0–104 d, Servos et al. 1992b)</td>
<td></td>
</tr>
<tr>
<td>4.13, 3.38</td>
<td>(guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)</td>
<td></td>
</tr>
<tr>
<td>4.13, 4.34, 4.38</td>
<td>(guppy, 21-d exposure, lipid wt basis: measured-Cn/Cn, calculated; rate constant ratio k1/k2 from nonlinear regression analysis, Loonen et al. 1994b)</td>
<td></td>
</tr>
<tr>
<td>3.38</td>
<td>(Poecilia reticulata, quoted, Devillers et al. 1996)</td>
<td></td>
</tr>
<tr>
<td>7.15, 8.45</td>
<td>(fish 5% lipid: BCFw/BCFl, Geyer et al. 2000)</td>
<td></td>
</tr>
<tr>
<td>8.02, 7.53</td>
<td>(fish muscle log BCFl calculated from water, sediment, Wu et al. 2001)</td>
<td></td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, log KOC:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.92</td>
<td>(estimated DOC partition coeff., Muir et al. 1985)</td>
<td></td>
</tr>
<tr>
<td>7.08</td>
<td>(organic carbon, calculated-QSAR, Fiedler &amp; Schramm 1990)</td>
<td></td>
</tr>
<tr>
<td>5.92</td>
<td>(DOC, De Voogt et al. 1990)</td>
<td></td>
</tr>
<tr>
<td>7.90</td>
<td>(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)</td>
<td></td>
</tr>
<tr>
<td>10.96</td>
<td>(sediment/water, quoted exptl., calculated-SOFA model, Govers &amp; Krop 1998)</td>
<td></td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatile:

Photolysis:

photolytic t½ = 16 h by both natural sunlight and fluorescent black light in hexane solution, (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)

solution photolysis t½ = 1460 min at 1.0 m from a GE Model RS sunlamp and surface photolysis of 46900 min on clean soft glass surface under the same conditions (Nestrick et al. 1980);

photolysis t½ = 24.3 h in hexadecane solution (Mamantov 1984)

photolysis k = 1.06 × 10⁻⁶ s⁻¹ in water acetonitrile (2:3, v/v) solution at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: t½ = 20.53 d in spring; t½ = 17.85 d in summer; t½ = 31.26 d in autumn; t½ = 50.45 d in winter; and t½ = 863 d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)

photolysis rate constant k = 1.06 × 10⁻⁶ s⁻¹ with t½ = 183.95 h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: k = 3.45 × 10² d⁻¹ with t½ = 21 d in spring, k = 3.97 × 10² d⁻¹ with t½ = 18 d in summer, k = 2.27 × 10² d⁻¹ with t½ = 31 d in fall, k = 1.40 × 10² d⁻¹ with t½ = 50 d in winter (Choudhary & Webster 1989)

photolysis decay rate constants when irradiated with UV light at 254 nm: k(calc) = 1.77 × 10⁻⁵ s⁻¹, 4.62 × 10⁻⁵ s⁻¹ for fly ash suspensions in distilled water, k(calc) = 1.42 × 10⁻⁵ s⁻¹ for fly ash suspensions in water-acetonitrile solution (2:3, v/v), and k(calc) = 2.74 × 10⁻⁵ s⁻¹ for fly ash suspensions in water-acetonitrile solution (2:3, v/v) with ozone (Muto et al. 1991);
Chlorinated Dibenzo-\(p\)-dioxins

Photolytic \(t_\text{\(\frac{1}{2}\)}\) = 37.3 h-native congener, \(t_\text{\(\frac{1}{2}\)}\) = 29.6 h for \(^{13}\)C-labeled congener in extract of fly ash and in tetradeclane solution (Tysklind & Rappe 1991);
photolysis \(k = 1.6 \times 10^{-3} \text{ min}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 440 \text{ min}\) in pure water, and \(k = 1.0 \times 10^{-3} \text{ min}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 680 \text{ min}\) in 60\% acetonitrile/water aqueous solutions at 300 nm (Kim & O’Keefe 2000);
photodegradation \(k = 0.12 \text{ h}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 5.8 \text{ h}\) when loaded on TiO\(_2\) film under UV (\(\lambda > 300 \text{ nm}\)) or solar light irradiation in the air (Choi et al. 2000).

\(t_\text{\(\frac{1}{2}\)} = 105 \text{ h}\) on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_\text{\(\text{OH}\)}\) for reaction with \(\text{OH}\) radical, \(k_\text{\(\text{NO}_3\)}\) with \(\text{NO}_3\) radical and \(k_\text{\(\text{O}_3\)}\) with \(\text{O}_3\) or as indicated, *data at other temperatures see reference:
\(k\) (oxidative degradation rate constant of water dissolved OCDD by ozone) is \(1.51 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}\) under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

\(k_\text{\(\text{OH}\)}(\text{calc}) = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) and a calculated tropospheric lifetime \(\tau = 9.6 \text{ d}\) based on gas phase \(\text{OH}\) reactions and a 12-h average daytime \(\text{OH}\) radical concentration of \(1.5 \times 10^6 \text{ molecule cm}^{-3}\) for OCDD at room temp. (Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants:
\(k_1 = 142 \text{ d}^{-1}\); \(k_2 = 0.053 \text{ d}^{-1}\) (fathead minnow, flow-through system, Muir et al. 1985; quoted, Adams et al. 1986)
\(k_1 = 11 \text{ d}^{-1}\); \(k_2 = 0.12 \text{ d}^{-1}\) (rainbow trout, flow-through system, Muir et al. 1985)
\(k_1 = 17, 5.0 \text{ d}^{-1}\); \(k_2 = 0.103, 0.142 \text{ d}^{-1}\) (rainbow trout exposed to concn of 20, 415 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
\(k_1 = 142 \text{ d}^{-1}\); \(k_2 = 0.053 \text{ d}^{-1}\) (fathead minnow exposed to concn of 9 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)
\(k_1 = 0.046 \text{ d}^{-1}\) (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
\(k_1 = 984 \text{ d}^{-1}\); \(k_2 = 1.4 \text{ d}^{-1}\) (guppy, Gobas & Schrap 1990)
\(k_1 = 60 \text{ d}^{-1}\); \(k_2 = 0.12 \text{ d}^{-1}\) (filter-feeder, Servos et al. 1992b)
\(k_1 = 30 \text{ d}^{-1}\); \(k_2 = 0.08 \text{ d}^{-1}\) (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)
\(k_1 = 275 \text{ L kg}^{-1} \text{ d}^{-1}\); \(k_2 = 119 \text{ d}^{-1}\) (guppy, 21-d exposure, wet wt base, Loonen et al. 1994)
\(k_2 = 0.0053 \text{ d}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 57 \text{ d}\) (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:
Air: atmospheric lifetime of \(\sim 7–8 \text{ h}\) for reaction with hydroxyl radicals (Atkinson 1987);
estimated reaction \(k = 0.0015 \text{ h}^{-1}\) (Paterson et al. 1990);
photodegradation \(t_\text{\(\frac{1}{2}\)} = 270 \text{ h}\) in a rotary photo-reactor adsorbed to clean silica gels by filtered \(\lambda < 290 \text{ nm}\) of light (Koester & Hites 1992);
tropospheric lifetime \(\tau = 9.6 \text{ d}\), calculated based on gas-phase reaction with \(\text{OH}\) radicals (Atkinson 1991); suggested \(t_\text{\(\frac{1}{2}\)} = 3950 \text{ h}\) at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000);
first-order photodegradation \(k = 0.12 \text{ h}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 5.8 \text{ h}\) when loaded on TiO\(_2\) film under UV (\(\lambda > 300 \text{ nm}\)) or solar light irradiation in the air (Choi et al. 2000).

Surface water: first order photolytic rate constant \(k <(0.3– 2.7) \times 10^{-3} \text{ h}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 7–16 \text{ h}\) exposed to sunlight in hexane solution (Dobbs & Grant 1979); direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: \(t_\text{\(\frac{1}{2}\)} = 20.53 \text{ in spring, } t_\text{\(\frac{1}{2}\)} = 17.85 \text{ in summer, } t_\text{\(\frac{1}{2}\)} = 31.26 \text{ in fall, } t_\text{\(\frac{1}{2}\)} = 50.45 \text{ d in winter and } t_\text{\(\frac{1}{2}\)} = 853.22 \text{ d averaged over full year (Choudhary & Webster 1986);}
\(k = 1.064 \times 10^{-4} \text{ s}^{-1}\) in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985a,1986); photolysis \(t_\text{\(\frac{1}{2}\)} = 183.95 \text{ h}\) in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct photolysis half-lives near water bodies at 40°N latitude: \(t_\text{\(\frac{1}{2}\)} = 21 \text{ d in spring, } t_\text{\(\frac{1}{2}\)} = 18 \text{ d in summer, } t_\text{\(\frac{1}{2}\)} = 31 \text{ d in fall and } t_\text{\(\frac{1}{2}\)} = 50 \text{ d in winter (Choudhary & Webster 1989);}
\(t_\text{\(\frac{1}{2}\)} = 4.0 \text{ d}\) in the water column of an experimental lake in northwestern Ontario (Servos et al. 1989); transformation \(k(\text{calc}) = 1.6 \times 10^{-3} \text{ h}^{-1}\) in simulated lake enclosure (Servos et al. 1992a); photolysis \(k = 1.6 \times 10^{-3} \text{ min}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 440 \text{ min}\) in pure water, and \(k = 1.0 \times 10^{-3} \text{ min}^{-1}\) with \(t_\text{\(\frac{1}{2}\)} = 680 \text{ min}\) in 60\% acetonitrile/water aqueous solutions at 300 nm (Kim & O’Keefe 2000);
suggested $t_{1/2} = 79000 \text{ h at } 7^\circ\text{C}$ for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:
Sediment: estimated reaction $k = (5.0 \times 10^{-3} - 1.0 \times 10^{-6}) \text{ h}^{-1}$ (Paterson et al. 1990);
$t_{1/2}(\text{calc}) = 10 \text{ yr with a transformation rate constant } k = 7.9 \times 10^{-6} \text{ h}^{-1}$ (Servos et al. 1992a)
$t_{1/2} = 0.2 - 142 \text{ yr}$ (Geyer et al. 2000)
degradation $t_{1/2} = 20 - 200 \text{ yr in sediment for all homologues}$ (estimated, Suzuki et al. 2000)
suggested $t_{1/2} = 130000 \text{ h at } 7^\circ\text{C for Baltic Proper environments}$ (Sinkkonen & Passivirta 2000).

Soil: undergoes photoreduction on soil surfaces to lower chlorinated congeners (Kieatiwong et al. 1990);
estimated reaction $k = 7.0 \times 10^{-7} \text{ h}^{-1}$ (Paterson et al. 1990)
$t_{1/2} > 10 \text{ yr}$ (Geyer et al. 2000)
degradation $t_{1/2} = 10 - 100 \text{ yr in soil}$ (estimated, Suzuki et al. 2000)
suggested $t_{1/2} = 130000 \text{ h at } 7^\circ\text{C for Baltic Proper environments}$ (Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} \sim 21 \text{ d from rat}$ (Norback et al. 1975; quoted, Birnbaum 1985);
elimination $t_{1/2} = 13.9 \text{ d for fathead minnow}$ (Muir et al. 1985, Adams et al. 1986);
elimination $t_{1/2} = 5 - 13 \text{ d for both rainbow trout and fathead minnow}$ (Muir et al. 1986);
mean biological $t_{1/2} \sim 15 \text{ d in rainbow trout}$ (Niimi 1986);
t$_{1/2} = 15 \text{ d in rainbow trout}$ (Niimi & Oliver 1986; quoted, Muir et al. 1986, 1990);
t$_{1/2} = 57 \text{ d in blue mussel for 99-d exposure experiment}$ (Hektoen et al. 1994).

## TABLE 8.1.1.26.1
Reported aqueous solubilities of octachlorodibenzo-$p$-dioxin at various temperatures

<table>
<thead>
<tr>
<th>$t/°\text{C}$</th>
<th>$S/\text{g·m}^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Webster et al. 1985 generator column-HPLC/LSC</td>
<td>20</td>
</tr>
<tr>
<td>Friesen et al. 1985 generator column-HPLC/LSC</td>
<td>20</td>
</tr>
<tr>
<td>Doucette &amp; Andren 1988a generator column-GC/ECD</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>60</td>
</tr>
<tr>
<td></td>
<td>80</td>
</tr>
</tbody>
</table>

$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 74.5$

at $40-80 \, ^\circ\text{C}$

**FIGURE 8.1.1.26.1** Logarithm of mole fraction solubility versus reciprocal temperature for octachlorodibenzo-$p$-dioxin.
### TABLE 8.1.1.26.2
Reported vapor pressures of octachlorodibenzo-\(p\)-dioxin at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C \log (T/K)
\end{align*}
\]

- log \(P = A - B/(T/K)\) (1)
- ln \(P = A - B/(T/K)\) (1a)
- log \(P = A - B/(C + t/°C)\) (2)
- ln \(P = A - B/(C + t/°C)\) (2a)
- log \(P = A - B/(C + T/K)\) (3)
- log \(P = A - B/(T/K) - C \log (T/K)\) (4)

<table>
<thead>
<tr>
<th>T/°C</th>
<th>(P/Pa)</th>
<th>T/°C</th>
<th>(P/Pa)</th>
<th>T/°C</th>
<th>(P/Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.1 × 10^{-10}</td>
<td>120.1</td>
<td>0.000280</td>
<td>175</td>
<td>0.0912</td>
</tr>
<tr>
<td>50</td>
<td>1.3 × 10^{-8}</td>
<td>124.9</td>
<td>0.000447</td>
<td>180</td>
<td>0.141</td>
</tr>
<tr>
<td>75</td>
<td>7.2 × 10^{-7}</td>
<td>129.9</td>
<td>0.000737</td>
<td>185</td>
<td>0.204</td>
</tr>
<tr>
<td>100</td>
<td>2.4 × 10^{-5}</td>
<td>134.9</td>
<td>0.00125</td>
<td>190</td>
<td>0.291</td>
</tr>
<tr>
<td>125</td>
<td>5.1 × 10^{-4}</td>
<td>139.9</td>
<td>0.00209</td>
<td>195</td>
<td>0.416</td>
</tr>
<tr>
<td></td>
<td></td>
<td>144.8</td>
<td>0.00352</td>
<td>200</td>
<td>0.607</td>
</tr>
<tr>
<td></td>
<td></td>
<td>149.8</td>
<td>0.00581</td>
<td>205</td>
<td>0.838</td>
</tr>
<tr>
<td></td>
<td></td>
<td>154.7</td>
<td>0.00949</td>
<td>210</td>
<td>1.20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>159.7</td>
<td>0.0153</td>
<td>215</td>
<td>1.67</td>
</tr>
<tr>
<td></td>
<td></td>
<td>165.0</td>
<td>0.0253</td>
<td>220</td>
<td>2.32</td>
</tr>
<tr>
<td></td>
<td></td>
<td>170.0</td>
<td>0.0406</td>
<td>225</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>175.0</td>
<td>0.0654</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>180.0</td>
<td>0.1023</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>185.0</td>
<td>0.1585</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>189.8</td>
<td>0.2515</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>194.7</td>
<td>0.383</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>199.7</td>
<td>0.584</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 86.7)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 151.13)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 61.4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 102)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 149.822)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### FIGURE 8.1.1.26.2
Logarithm of vapor pressure versus reciprocal temperature for octachlorodibenzo-\(p\)-dioxin.

© 2006 by Taylor & Francis Group, LLC
## TABLE 8.2.1
Summary of physical properties of some chlorinated dioxins

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW (g/mol)</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, ( F ) at 25°C*</th>
<th>Molar volume, ( V_m ) cm³/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibenzo-( p )-dioxin</td>
<td>262-12-4</td>
<td>( C_{12}H_8O_2 )</td>
<td>184.191</td>
<td>120.5</td>
<td>0.116</td>
<td>143.82</td>
<td>177.0</td>
</tr>
<tr>
<td>1-Chloro-</td>
<td>39227-53-7</td>
<td>( C_{12}H_7O_2Cl )</td>
<td>218.636</td>
<td>105.5</td>
<td>0.162</td>
<td>157.41</td>
<td>197.9</td>
</tr>
<tr>
<td>2-Chloro-</td>
<td>39227-54-8</td>
<td>( C_{12}H_7O_2Cl )</td>
<td>218.636</td>
<td>89</td>
<td>0.236</td>
<td>154.85</td>
<td>197.9</td>
</tr>
<tr>
<td>2,3-Dichloro-</td>
<td>29446-15-9</td>
<td>( C_{12}H_6O_2Cl_2 )</td>
<td>253.081</td>
<td>164</td>
<td>358</td>
<td>0.0433</td>
<td>164.07</td>
</tr>
<tr>
<td>2,7-Dichloro-</td>
<td>33857-26-0</td>
<td>( C_{12}H_6O_2Cl_2 )</td>
<td>253.081</td>
<td>201</td>
<td>374.5</td>
<td>0.0188</td>
<td>165.88</td>
</tr>
<tr>
<td>2,8-Dichloro-</td>
<td>38964-22-6</td>
<td>( C_{12}H_6O_2Cl_2 )</td>
<td>253.081</td>
<td>151</td>
<td>0.0580</td>
<td>165.88</td>
<td>218.8</td>
</tr>
<tr>
<td>1,2,4-Trichloro-</td>
<td>39227-58-2</td>
<td>( C_{12}H_6O_2Cl_3 )</td>
<td>287.526</td>
<td>129</td>
<td>375</td>
<td>0.0954</td>
<td>179.66</td>
</tr>
<tr>
<td>1,3,7-Trichloro-</td>
<td>67026-17-5</td>
<td>( C_{12}H_6O_2Cl_3 )</td>
<td>287.526</td>
<td>148.5</td>
<td>398</td>
<td>0.0614</td>
<td>179.11</td>
</tr>
<tr>
<td>2,3,7-Trichloro-</td>
<td>33857-28-2</td>
<td>( C_{12}H_6O_2Cl_3 )</td>
<td>287.526</td>
<td>162–163</td>
<td>408.4</td>
<td>0.0448</td>
<td>175.10</td>
</tr>
<tr>
<td>1,2,3,4-Tetrachloro-</td>
<td>30746-58-8</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>189</td>
<td>419</td>
<td>0.0246</td>
<td>186.71</td>
</tr>
<tr>
<td>1,2,3,7-Tetrachloro-</td>
<td>67028-18-6</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>172</td>
<td>438.3</td>
<td>0.0361</td>
<td>186.52</td>
</tr>
<tr>
<td>1,2,7,8-Tetrachloro-</td>
<td>34816-53-0</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>321.971</td>
<td>219</td>
<td>438.3</td>
<td>0.0125</td>
</tr>
<tr>
<td>1,3,6,8-Tetrachloro-</td>
<td>30746-58-8</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>193.5–195</td>
<td>438.3</td>
<td>0.0218</td>
<td>188.33</td>
</tr>
<tr>
<td>1,3,7,8-Tetrachloro-</td>
<td>50585-46-1</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>193.5–195</td>
<td>438.3</td>
<td>0.0218</td>
<td>188.33</td>
</tr>
<tr>
<td>1,3,7,9-Tetrachloro-</td>
<td>64270-53-5</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>193.5–195</td>
<td>438.3</td>
<td>0.0218</td>
<td>188.33</td>
</tr>
<tr>
<td>1,3,7,8-Tetrachloro-</td>
<td>1746-01-6</td>
<td>( C_{12}H_5O_2Cl_4 )</td>
<td>321.971</td>
<td>295</td>
<td>0.00224</td>
<td>184.32</td>
<td>260.6</td>
</tr>
<tr>
<td>1,2,3,4,7-Pentachloro-</td>
<td>39227-61-7</td>
<td>( C_{12}H_5O_2Cl_5 )</td>
<td>356.416</td>
<td>195</td>
<td>464.7</td>
<td>0.0215</td>
<td>197.74</td>
</tr>
<tr>
<td>1,2,3,7,8-Pentachloro-</td>
<td>40321-76-4</td>
<td>( C_{12}H_5O_2Cl_5 )</td>
<td>356.416</td>
<td>464.7</td>
<td>195</td>
<td>464.7</td>
<td>0.0168</td>
</tr>
<tr>
<td>1,2,4,7,8-Pentachloro-</td>
<td>58802-08-7</td>
<td>( C_{12}H_5O_2Cl_5 )</td>
<td>356.416</td>
<td>206</td>
<td>464.7</td>
<td>0.0168</td>
<td>199.91</td>
</tr>
<tr>
<td>1,2,3,4,7,8-Hexachloro-</td>
<td>39227-26-8</td>
<td>( C_{12}H_5O_2Cl_6 )</td>
<td>390.861</td>
<td>273</td>
<td>487.7</td>
<td>0.00369</td>
<td>206.96</td>
</tr>
<tr>
<td>1,2,3,6,7,8-Hexachloro-</td>
<td>57653-85-7</td>
<td>( C_{12}H_5O_2Cl_6 )</td>
<td>390.861</td>
<td>285</td>
<td>487.7</td>
<td>0.00281</td>
<td>207.16</td>
</tr>
<tr>
<td>1,2,3,7,8,9-Hexachloro-</td>
<td>19408-74-3</td>
<td>( C_{12}H_5O_2Cl_6 )</td>
<td>390.861</td>
<td>243–244</td>
<td>487.7</td>
<td>0.00718</td>
<td>207.16</td>
</tr>
<tr>
<td>1,2,4,6,7,9-Hexachloro-</td>
<td>39227-62-8</td>
<td>( C_{12}H_5O_2Cl_6 )</td>
<td>390.861</td>
<td>238–240</td>
<td>487.7</td>
<td>0.00795</td>
<td>215.50</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-Heptachloro-</td>
<td>35822-46-9</td>
<td>( C_{12}H_5O_2Cl_7 )</td>
<td>425.308</td>
<td>265</td>
<td>507.2</td>
<td>0.00442</td>
<td>218.38</td>
</tr>
<tr>
<td>1,2,3,4,7,8,9-Heptachloro-</td>
<td>3268-87-9</td>
<td>( C_{12}H_5O_2Cl_7 )</td>
<td>425.308</td>
<td>507.2</td>
<td>0.00442</td>
<td>218.38</td>
<td>323.3</td>
</tr>
<tr>
<td>Octachloro-</td>
<td>3268-87-9</td>
<td>( C_{12}H_5O_2Cl_8 )</td>
<td>459.751</td>
<td>331</td>
<td>510</td>
<td>0.000995</td>
<td>229.60</td>
</tr>
</tbody>
</table>

*Assuming \( \Delta S_m = 56 \text{ J/mol K} \); (a) Govers et al. 1990 (at 25°C).
### TABLE 8.2.2
Selected physical-chemical properties of some chlorinated dioxins at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PS/Pa</td>
<td>PL/Pa</td>
<td>S/(mg/m³)</td>
</tr>
<tr>
<td>Dibenzo-p-dioxin</td>
<td>0.055</td>
<td>0.474</td>
<td>865</td>
</tr>
<tr>
<td>1-CDD</td>
<td>0.012</td>
<td>0.074</td>
<td>417</td>
</tr>
<tr>
<td>2-CDD</td>
<td>0.017</td>
<td>0.0730</td>
<td>295</td>
</tr>
<tr>
<td>2,3-DCDD</td>
<td>0.00039</td>
<td>0.00901</td>
<td>14.9</td>
</tr>
<tr>
<td>2,7-DCDD</td>
<td>0.00012</td>
<td>0.00811</td>
<td>3.75</td>
</tr>
<tr>
<td>2,8-DCDD</td>
<td>0.00014</td>
<td>0.00241</td>
<td>16.7</td>
</tr>
<tr>
<td>1,2,4-T₃CDD</td>
<td>0.0001</td>
<td>0.00105</td>
<td>8.41</td>
</tr>
<tr>
<td>1,2,3,4-T₄CDD</td>
<td>6.40 × 10⁻⁶</td>
<td>2.60 × 10⁻⁴</td>
<td>0.55</td>
</tr>
<tr>
<td>1,2,3,7-T₄CDD</td>
<td>1.00 × 10⁻⁶</td>
<td>2.77 × 10⁻⁵</td>
<td>0.42</td>
</tr>
<tr>
<td>1,3,6,8-T₄CDD</td>
<td>7.00 × 10⁻⁷</td>
<td>5.60 × 10⁻⁵</td>
<td>0.32</td>
</tr>
<tr>
<td>2,3,7,8-T₄CDD</td>
<td>2.00 × 10⁻⁷</td>
<td>8.93 × 10⁻⁵</td>
<td>0.0193</td>
</tr>
<tr>
<td>1,2,3,4,7-P₅CDD</td>
<td>8.80 × 10⁻⁸</td>
<td>4.09 × 10⁻⁶</td>
<td>0.118</td>
</tr>
<tr>
<td>1,2,3,4,7,8-H₆CDD</td>
<td>5.10 × 10⁻⁹</td>
<td>1.38 × 10⁻⁶</td>
<td>0.006</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-H₇CDD</td>
<td>7.50 × 10⁻¹⁰</td>
<td>1.70 × 10⁻⁷</td>
<td>0.0024</td>
</tr>
<tr>
<td>OCDD</td>
<td>1.10 × 10⁻¹⁰</td>
<td>1.11 × 10⁻⁷</td>
<td>0.000074</td>
</tr>
</tbody>
</table>
### TABLE 8.2.3
Suggested half-life classes of polychlorinated dibenzo-\(p\)-dioxins in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibeno-(p)-dioxin</td>
<td>3</td>
<td>3</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>2-CDD</td>
<td>4</td>
<td>4</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>2,7-DCDD</td>
<td>4</td>
<td>4</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>2,8-DCDD</td>
<td>4</td>
<td>4</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,4-T(_3)CDD</td>
<td>4</td>
<td>4</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1,2,3,4-T(_4)CDD</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>2,3,7,8-T(_4)CDD</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>1,2,3,4,7-P(_5)CDD</td>
<td>5</td>
<td>5</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>1,2,3,4,7,8-H(_6)CDD</td>
<td>5</td>
<td>6</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-H(_7)CDD</td>
<td>5</td>
<td>6</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>OCDD</td>
<td>5</td>
<td>7</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

where,

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>&lt; 10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~ 1 day)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~ 2 days)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1,700 (~ 2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5,500 (~ 8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17,000 (~ 2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55,888 (~ 6 years)</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>

**FIGURE 8.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-\(p\)-dioxins.
FIGURE 8.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-\(p\)-dioxins.

FIGURE 8.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzo-\(p\)-dioxins.
FIGURE 8.2.4 Henry’s law constant versus Le Bas molar volume for polychlorinated dibenzo-p-dioxins.

FIGURE 8.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzo-p-dioxins.
8.3 REFERENCES


Choudhary, G.G., Webster, G.R.B. (1989) Environmental photochemistry of OCDDs. 2. Quantum yields of the direct phototransformation of 1,2,3,7-tetra-, 1,3,6,8-tetra-, 1,2,3,4,6,7,8-hepta-, and 1,2,3,4,6,7,8,9-octachloro-dibenzo-p-dioxin in aqueous acetonitrile and their sunlight half-lives. *J. Agric. Food Chem.* 37, 254–251.


Chlorinated Dibenzo-p-dioxins


Rordorf, B.F. (1986a) Private communication, Ciba Geigy Ltd., Switzerland.


Sangster, J. (1993) LOGKOW Databank, Sangster Research Laboratories, Montreal, Quebec, Canada.


9 Chlorinated Dibenzofurans

CONTENTS

9.1 List of Chemicals and Data Compilations .......................................................... 2168
  9.1.1 Dibenzofuran and chlorinated dibenzofurans ............................................. 2168
    9.1.1.1 Dibenzofuran ..................................................................................... 2168
    9.1.1.2 2-Chlorodibenzofuran ..................................................................... 2173
    9.1.1.3 3-Chlorodibenzofuran ..................................................................... 2175
    9.1.1.4 2,3-Dichlorodibenzofuran ............................................................... 2177
    9.1.1.5 2,7-Dichlorodibenzofuran ............................................................... 2179
    9.1.1.6 2,8-Dichlorodibenzofuran ............................................................... 2181
    9.1.1.7 3,6-Dichlorodibenzofuran ............................................................... 2184
    9.1.1.8 2,3,8-Trichlorodibenzofuran ............................................................. 2186
    9.1.1.9 2,4,6-Trichlorodibenzofuran ............................................................. 2188
    9.1.1.10 2,4,8-Trichlorodibenzofuran ............................................................ 2190
    9.1.1.11 1,2,3,4-Tetrachlorodibenzofuran ..................................................... 2193
    9.1.1.12 1,2,3,7-Tetrachlorodibenzofuran ..................................................... 2195
    9.1.1.13 1,2,7,8-Tetrachlorodibenzofuran ..................................................... 2197
    9.1.1.14 1,3,6,8-Tetrachlorodibenzofuran ..................................................... 2199
    9.1.1.15 1,3,7,8-Tetrachlorodibenzofuran ..................................................... 2201
    9.1.1.16 1,3,7,9-Tetrachlorodibenzofuran ..................................................... 2203
    9.1.1.17 2,3,7,8-Tetrachlorodibenzofuran ..................................................... 2205
    9.1.1.18 1,2,3,4,7-Pentachlorodibenzofuran .................................................. 2209
    9.1.1.19 1,2,3,7,8-Pentachlorodibenzofuran .................................................. 2211
    9.1.1.20 1,2,4,7,8-Pentachlorodibenzofuran .................................................. 2213
    9.1.1.21 2,3,4,7,8-Pentachlorodibenzofuran .................................................. 2215
    9.1.1.22 1,2,3,4,6,8-Hexachlorodibenzofuran .............................................. 2218
    9.1.1.23 1,2,3,4,7,8-Hexachlorodibenzofuran .............................................. 2220
    9.1.1.24 1,2,3,6,7,8-Hexachlorodibenzofuran .............................................. 2223
    9.1.1.25 1,2,3,7,8,9-Hexachlorodibenzofuran .............................................. 2226
    9.1.1.26 1,2,4,6,7,8-Hexachlorodibenzofuran .............................................. 2228
    9.1.1.27 1,2,4,6,8,9-Hexachlorodibenzofuran .............................................. 2230
    9.1.1.28 2,3,4,6,7,8-Hexachlorodibenzofuran .............................................. 2232
    9.1.1.29 1,2,3,4,6,7,8-Heptachlorodibenzofuran ........................................... 2234
    9.1.1.30 1,2,3,4,6,8,9-Heptachlorodibenzofuran .......................................... 2237
    9.1.1.31 1,2,3,4,7,8,9-Heptachlorodibenzofuran .......................................... 2239
    9.1.1.32 Octachlorodibenzofuran .................................................................. 2242
  9.2 Summary Tables and QSAR Plots ...................................................................... 2247
  9.3 References ...................................................................................................... 2253
9.1 LIST OF CHEMICALS AND DATA COMPILATIONS

9.1.1 DIBENZOFURAN AND CHLORINATED DIBENZOFURANS

9.1.1.1 Dibenzofuran

Common Name: Dibenzofuran
Synonym: diphenylene oxide
Chemical Name: dibenzofuran
CAS Registry No: 132-64-9
Molecular Formula: C_{12}H_8O, C_6H_4OC_6H_4
Molecular Weight: 168.191
Melting Point (°C):
86.5 (Lide 2003)
Boiling Point (°C):
287 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.0886 (99°C, Weast 1982–83)
Molar Volume (cm³/mol):
154.4 (99°C, calculated-density, Stephenson & Malanowski 1987)
147.8 (Ruelle & Kesselring 1997)
176.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆H_v (kJ/mol):
65.4 (Rordorf 1989)
Enthalpy of Sublimation, ∆H_{subl} (kJ/mol):
85.63 (Rordorf 1989)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
19.6 (Rordorf 1987, 1989; quoted, Ruelle & Kesselring 1997)
18.6 (Chickos et al. 1999)
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.249 (mp at 86.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3.11 (Lu et al. 1978)
10.03 (shake flask-HPLC/UV, Banerjee et al. 1980)
6.56 (selected average, Pearlman et al. 1984)
4.22* (generator column-GC, measured range 4–39.8°C, Doucette & Andren 1988a)
S/(mol/L) = 8.32 × 10^{-6} \exp(0.041·t°C); temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a); or
log x = −1558/(T/K) − 1.135; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
3.36 (calculated-TSA, Dickhut et al. 1994)
4.30 (computed-expert system SPARC, Kollig 1995)
4.75* ± 0.22 (generator column-HPLC/UV, Shiu et al. 1997)
4.69 ± 0.18 (shake flask-GC, Shiu et al. 1997)
2.43 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle Kesselring 1997)
17.21; 62.49 (supercooled liquid S_{lj}, quoted lit. average; calculated-SOFA-Solubility parameters for Fate Analysis model, Govers & Krop 1998)
ln x = −1.6385 − 3842.2/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
Chlorinated Dibenzofurans

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.276* (gas saturation, extrapolated-Antoine eq. from exptl. data, measured temp range, 30–70°C, Hansen & Eckert 1986)

0.506* (26°C, gas saturation exptl. data, measured range 49–74°C, Sato et al. 1986)

0.466 (gas saturation-GC, extrapolated-Antoine eq. derived from exptl. data, temp range 49–74°C, Sato et al. 1986)

0.35* (gas saturation-GC, measured range 25–125°C Rordorf 1986, 1989)

2.026 (extrapolated liquid value P_L, Antoine eq., Stephenson & Malanowski 1987)

\[ \log \left( \frac{P}{\text{kPa}} \right) = 5.8968 - \frac{1851.27}{(-82.64 + T/K)} \]; temp range 403–559 K (Antoine eq., Stephenson & Malanowski 1987)

0.40 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 17.6646 - 3.1989 \times 10^3/(T/K) - 3.3346 \log(T/K) + 6.0686 \times 10^{-10} \times (T/K) + 4.4676 \times 10^{-7} \times (T/K)^2; \] temp range 356–838 K (vapor pressure eq., Yaws et al. 1994)

0.360 (computed-expert system SPARC, Kollig 1995)

0.708; 0.123 (supercooled liquid P_L, quoted exptl. or exptl. average; calculated-SOFA model (Solubility parameters of Fate Analysis model), Govers & Krop 1998)

\[ \log \left( \frac{P}{\text{Pa}} \right) = 13.17192 - 4083/(T/K); \text{temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)} \]

0.429 (gas saturation-HPLC/fluorescence, de Seze et al. 2000)

0.398* (25.2°C, Knudsen effusion method, measured range 20.2–45°C Li et al. 2002)

\[ \ln \left( \frac{P}{\text{Pa}} \right) = 33.54 - 10313/(T/K); \text{temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2002 2004)} \]

\[ \ln \left( \frac{P}{\text{Pa}} \right) = (32.203 \pm 0.576) - (9880.4 \pm 176)/(T/K); \text{temp range 295–318 K (Knudsen effusion technique, Li et al. 2004)} \]

Henry’s Law Constant (Pa m^3/mol at 25°C):

14.16 (calculated-P/C with selected values)

14.20 (computed-expert system SPARC, Kollig 1995)


Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.12 (HPLC-RT correlation, Veith et al. 1979a)

4.12 (Hansch & Leo 1979)

4.17 (shake flask-HPLC/UV, Banerjee et al. 1980)

3.91, 4.12, 4.18; 3.96, 4.10, 4.17 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)

3.92 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)

4.31 (generator column-GC/ECD, both phases, Doucette & Andren 1987)

3.86 (HPLC-RT correlation, Doucette & Andren 1988b)

4.21, 3.81 (shake flask-HPLC, TLC-RT correlation, De Voogt et al. 1990)

4.12 (recommended, Sangster 1993)

4.12 (recommended, Hansch et al. 1995)

4.27 (generator column-HPLC/UV, Shiu et al. 1997)

4.273* (shake flask-HPLC/UC, measured S_0 and S_w, Shiu et al. 1997)

4.09 ± 0.19, 4.12 ± 0.63; 4.12 (HPLC-k’ correlation: ODS-65 column, Diol-35 column; quoted lit average value, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.13 (fathead minnow, 28 d exposure, Veith et al. 1979b)

3.13, 2.80 (quoted exptl., calculated-K_{OW}, Mackay 1982)

3.13, 3.13 (quoted exptl., calculated-MCI \chi, Sabljic 1987)
3.13 (calculated-\(K_{\text{OW}}\), Isnard & Lambert 1989)
3.68; 4.08 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, \(\log K_{\text{OC}}\):
3.80 (computed-\(K_{\text{OW}}\), Kollig 1995)
4.15 (humic acid, HPLC-\(k'\) correlation, Nielsen et al. 1997)
3.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.84 (soil-pore-water partition coeff. for Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
Volatilization:
Photolysis:
Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO}_3}\) with NO3 radical and \(k_{\text{O}_3}\) with \(O_3\) or as indicated, *data at other temperatures see reference:
\[
k_{\text{OH}} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ corresponding to an atmospheric lifetime of about 8 h (Atkinson 1987a)}
\]
\[k_{\text{OH}} = 3.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Atkinson 1987b)}
\]
\[t_{1/2} = 1.9–19 \text{ h based on estimated rate constant with OH radicals in air (Howard 1991)}
\]
\[k_{\text{OH}} = 3.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule cm}^{-3}, \text{ the tropospheric lifetime was calculated to be 0.5 d (Atkinson 1991)}
\]
\[k_{\text{OH}} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime of 3.7 d; } k_{\text{NO}_3} < 7 \times 10^{-30} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with } O_3 \text{ with calculated tropospheric lifetime } >250 \text{ d at room temp. (Kwok et al. 1994)}
\]
\[k_{\text{OH}(\text{exptl})} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{OH}(\text{calc})} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ corresponding to a tropospheric lifetime of 3.7 d at room temp. (Kwok et al. 1995)}
\]
Hydrolysis:
Biodegradation: biodegradation \(t_{1/2}\) ~168–672 h and anaerobic \(t_{1/2}\) = 672–2688 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991); nonautoclaved groundwater samples at hazardous waste site with a concentration of approximate 0.09 mg/L are degraded by microbes at rates about 30% per week while the levels of the controls decreased only about half that rate (Lee et al. 1984).
Biotransformation:
Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants:

Half-Lives in the Environment:
Air: the calculated atmospheric lifetime range from ~60–120 h (Atkinson 1987a);
\[t_{1/2} = 1.9–19 \text{ h, based on estimated rate constants for reaction with OH radicals (Howard et al. 1991)}; \]
the tropospheric lifetime was calculated 0.5 d for the gas-phase reaction for OH radicals using a 12-h average daytime OH radical concn of 1.5 \times 10^6 (Atkinson 1991);
calculated room temp. tropospheric lifetimes of 3.7 d for reaction with OH radical, >7 yr with NO3 radical, and >250 d for reaction with O3 (Kwok et al. 1994);
room temp. tropospheric lifetime was calculated to be 3.7 d for reaction with OH radical (Kwok et al. 1995).
Surface water: \(t_{1/2}\) =168–672 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).
Groundwater: \(t_{1/2}\) = 205–835 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).
Sediment:
Soil: \(t_{1/2}\) = 168–672 h, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).
Biota:
### TABLE 9.1.1.1
Reported aqueous solubilities and octanol-water partition coefficients of dibenzofuran at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>Octanol-water partition coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-HPLC/UV</td>
<td>generator column-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
</tr>
<tr>
<td>5</td>
<td>1.914</td>
<td>3.9</td>
</tr>
<tr>
<td>15</td>
<td>3.004</td>
<td>25</td>
</tr>
<tr>
<td>25</td>
<td>4.75</td>
<td>39.8</td>
</tr>
<tr>
<td>35</td>
<td>7.56</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>11.8</td>
<td></td>
</tr>
</tbody>
</table>

shake flask-HPLC/UV
25 4.69

$$\Delta H_{sol}/(kJ \ mol^{-1}) = 33.3$$ for 5–45°C

![Solubility vs. 1/T](image1)

![K₉₀₈ vs. 1/T](image2)

**FIGURE 9.1.1.1** Logarithm of mole fraction solubility and K₉₀₈ versus reciprocal temperature for dibenzofuran.
TABLE 9.1.1.2
Reported vapor pressures of dibenzofuran at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) & \quad \ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) & \quad \ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Hanson &amp; Eckert 1986</th>
<th>Sato et al. 1986</th>
<th>Rordorf 1989</th>
<th>Li et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>gas saturation-IR</td>
<td>gas saturation-electrobalance</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>30</td>
<td>0.4874</td>
<td>25.85</td>
<td>0.506</td>
</tr>
<tr>
<td>35</td>
<td>0.7818</td>
<td>35.85</td>
<td>1.48</td>
</tr>
<tr>
<td>40</td>
<td>1.280</td>
<td>40.75</td>
<td>2.35</td>
</tr>
<tr>
<td>45</td>
<td>2.128</td>
<td>45.85</td>
<td>3.71</td>
</tr>
<tr>
<td>50</td>
<td>3.200</td>
<td>52.45</td>
<td>6.69</td>
</tr>
<tr>
<td>55</td>
<td>4.679</td>
<td>55.65</td>
<td>8.5</td>
</tr>
<tr>
<td>60</td>
<td>7.246</td>
<td>59.75</td>
<td>12.5</td>
</tr>
<tr>
<td>65</td>
<td>12.78</td>
<td>60.35</td>
<td>13.5</td>
</tr>
<tr>
<td>70</td>
<td>19.71</td>
<td>64.45</td>
<td>18.3</td>
</tr>
<tr>
<td></td>
<td>65.05</td>
<td>19.9</td>
<td></td>
</tr>
<tr>
<td>log (P/Pa) = B - A/(T/K) = 66.15</td>
<td>21.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>16.30</td>
<td>68.75</td>
<td>26.1</td>
</tr>
<tr>
<td>B</td>
<td>4132</td>
<td>69.35</td>
<td>27.1</td>
</tr>
<tr>
<td>\Delta H_{subl}/(kJ mol^{-1}) = 79.1</td>
<td>72.75</td>
<td>35.4</td>
<td></td>
</tr>
</tbody>
</table>

eq. 3 P/Pa
A 22.1098
B 4707.68
C -92.332

FIGURE 9.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for dibenzofuran.
9.1.1.2 2-Chlorodibenzofuran

![Chemical Structure](#)

**Common Name:** 2-Chlorodibenzofuran  
**Synonym:** 2-MCDF  
**Chemical Name:** 2-Chlorodibenzofuran  
**CAS Registry No:** 51230-49-0  
**Molecular Formula:** C_{12}H_{7}ClO, C_{6}H_{4}OC_{6}H_{3}Cl  
**Molecular Weight:** 202.637  
**Melting Point (°C):**  
101.5–102.5 (Rordorf 1989)  
**Boiling Point (°C):**  
338.2 (Rordorf 1989)  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 197.6 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, ∆H_v (kJ/mol):** 75.2 (Rordorf 1989)  
**Enthalpy of Sublimation, ∆H_{subl} (kJ/mol):** 95.28 (Rordorf 1989)  
**Enthalpy of Fusion, ∆H_{fus} (kJ/mol):** 19.4 (Rordorf 1987, 1989)  
**Entropy of Fusion, ∆S_{fus} (J/mol K):** 52 (Rordorf 1986, 1987, 1989)  
**Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:**  
**Water Solubility (g/m³ or mg/L at 25°C):**  
11.66 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)  
**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
9.6 × 10⁻³, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)  
0.537 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)  
log (P_L/mmHg) = 40.57 – 5556/(T/K) – 9.999·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)  
0.174; 0.537 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
9.12 (calculated-SOFA model, Govers & Krop 1998)  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
4.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)  
5.15; 4.37 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)  
**Octanol/Air Partition Coefficient, log K_{oa}:**  
**Bioconcentration Factor, log BCF or log K_b:**  
4.51 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)  
4.77; 4.51 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, log $K_{OC}$:
- 4.38 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (16–22) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
  - $k_{OH}(calc) = (5.0–5.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);
  - calculated tropospheric lifetime was 2.9 d for the gas-phase reaction with OH radical (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:
Common Name: 3-Chlorodibenzofuran
Synonym: 3-MCDF
Chemical Name: 3-Chlorodibenzofuran
CAS Registry No: 25074-67-3
Molecular Formula: C_{12}H_{7}ClO, C_{6}H_{4}OC_{6}H_{3}Cl
Molecular Weight: 202.637
Melting Point (°C):
101–102 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
338.2 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
197.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
75.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
95.313 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
12.21 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
6.34; 12.21 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.970, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
0.490 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
log (P_L/mmHg) = 40.57 – 5553/(T/K) – 9.999·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
0.174; 0.490 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
7.76 (calculated-SOFA model, Govers & Krop 1998)
10.23; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log K_{ow}:
4.35 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.15; 4.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{bi}:
4.53 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
4.77; 4.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, log $K_{OC}$:
- 4.34 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 3.96; 4.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference:

$k_{OH} = (16–22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH(calc)} = (5.0–5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);

calculated tropospheric lifetime of 2.9 d for with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
9.1.1.4 2,3-Dichlorodibenzofuran

Common Name: 2,3-Dichlorodibenzofuran
Synonym: 2,3-DCBF
Chemical Name: 2,3-dichlorodibenzofuran
CAS Registry No: 64126-86-9
Molecular Formula: C₆H₃ClOC₆H₃Cl
Molecular Weight: 237.082
Melting Point (°C):
125.5–127 (Rordorf 1989)
Boiling Point (°C):
375 (Rordorf 1989)
Density (g/cm³):
218.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
78.8 (Rordorf 1989)
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
105.04 (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
25.1 (Rordorf 1989)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), $F$:
Water Solubility (g/m³ or mg/L at 25°C):
1.50 (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
0.716; 1.50 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.50 × 10⁻⁴, 1.7 × 10⁻², 0.29, 3.20, 27.0 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
0.0282 (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
$\log (P_L/mmHg) = 39.20 – 5757/(T/K) – 9.466 \cdot \log (T/K)$ (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
0.1096; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
4.365 (calculated-SOFA model, Govers & Krop 1998)
4.79; 4.365 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log $K_{ow}$:
5.11 (calculated-SOFA model, Govers & Krop 1998)
5.43; 5.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log $K_{oa}$:
Bioconcentration Factor, log BCF or log $K_B$:
4.82 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.04; 4.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, $\log K_{OC}$:
- 5.39 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 5.15; 5.39 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:
- $k_{OH}$ = $(6.6–16) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
- $k_{OH}(calc) = (2.6–3.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);
- room temp. tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:
9.1.1.5 2,7-Dichlorodibenzofuran

Common Name: 2,7-Dichlorodibenzofuran
Synonym: 2,7-DCBF
Chemical Name: 2,7-dichlorodibenzofuran
CAS Registry No: 73992-98-6
Molecular Formula: C₆H₃ClOC₆H₃Cl
Molecular Weight: 237.082
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔH_sabl (kJ/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
2.32 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.785; 2.32 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0501 (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
log (P_L/mmHg) = 39.23 – 5755/(T/K) – 9.466·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
0.0123; 0.0501 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry’s Law Constant (Pa·m³/mol):
5.01 (calculated-SOFA model, Govers & Krop 1998)
4.90; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_ow:
5.02 (calculated-SOFA model, Govers & Krop 1998)
5.41; 5.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_oa:

Bioconcentration Factor, log BCF or log K_B:
4.79 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
5.03; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K OC:
5.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.10; 5.27 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis: photolysis k = 0.23 min⁻¹ with t½ = 3.0 min in pure water and k = 0.011 min⁻¹ with t½ = 63 min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor (Kim & O’Keefe 2000)
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (6.6–16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.6–3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical at room temp. (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
9.1.1.6 2,8-Dichlorodibenzofuran

Common Name: 2,8-Dichlorodibenzofuran
Synonym: 2,8-DCDF
Chemical Name: 2,8-dichlorodibenzofuran
CAS Registry No: 5409-83-6
Molecular Formula: C₆H₃ClOC₆H₃Cl
Molecular Weight: 237.082
Melting Point (°C):
184–185 (Kuroki et al. 1984)
Boiling Point (°C):
375 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
218.5 (calculated-Le Bas method at normal boiling point)
173.6 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
74.2 (Rordorf 1989)
Enthalpy of Sublimation, \( \Delta H_{sub} \) (kJ/mol):
101.423 (Rordorf 1989)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
25.1 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
18.6 (exptl., Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
55 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming \( \Delta S = 56 \) J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0145* (generator column-GC, measured range 4.5–39.5°C, Doucette & Andren 1988a)
S/(mol/L) = 1.24 \times 10^{-6} \exp(0.082-t°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
\[ \log x = -2344/(T/K) + 1.093; \text{ temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)} \]
0.024 (calculated-TSA, Dickhut et al. 1994)
0.0431 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
2.11 (supercooled liquid \( S_L \), calculated-SOFA model, Govers & Krop 1998)
\[ \ln x = -2.515 – 5398.4/(T/K); \text{ temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)} \]
0.75; 2.11 (supercooled liquid \( S_L \), GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9.6 \times 10^{-4} (estimated, van den Berg & Olie 1985)
3.9 \times 10^{-4*} (calculated-bp and \( \Delta H_{fus} \), Rordorf 1987, 1989)
0.0145; 0.0417 (supercooled liquid \( P_L \), quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
\[ \log (P/Pa) = 14.30669 – 5281.67/(T/K); \text{ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)} \]
0.0115; 0.0417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
1.06 \times 10^{-3} (solid \( P_S \), gas saturation-GC/MS, Mader & Pankow 2003)
0.0412 (supercooled liquid \( P_L \), calculated from \( P_S \) assuming \( \Delta S_{fus} = 56 \) J/mol K, Mader & Pankow 2003)
\[ \log (P_L/mmHg) = 39.21 – 5756/(T/K) – 9.466 \cdot \log (T/K) \text{ (supercooled liquid } P_L, \text{ Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)} \]
\[
\ln \left( \frac{P}{Pa} \right) = 32.943 - 12162/(T/K), \text{ temp range } 298-398 \text{ K (regression eq. of Rordorf 1989 data, Li et al. 2004)} \\
\ln \left( \frac{P}{Pa} \right) = (36.010 \pm 0.393) - (13262 \pm 144)/(T/K); \text{ temp range } 348-383 \text{ K (Knudsen effusion technique, Li et al. 2004)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C):

- 6.31; 4.57 (quoted lit.; calculated-SOFA model, Govers & Krop 1998)
- 4.79; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 5.56, 5.97, 6.16; 5.65, 5.95, 6.15 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
- 5.30 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
- 5.44 (generator column-GC/ECD, Doucette & Andren 1987)
- 5.12 (HPLC-RT correlation, Doucette & Andren 1988b)
- 5.65 (recommended, Sangster 1993)
- 5.65 (recommended, Hansch et al. 1995)
- 5.42 (GC-RI correlation; Wang & Wong 2003)

Octanol/Air Partition Coefficient, log \( K_{oa} \):

Bioconcentration Factor, log BCF:

- 5.04 (guppy, Loonen et al. 1994a)
- 5.04; 4.81 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
- 5.04; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log \( K_{oc} \):

- 5.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 5.13; 5.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatileization:
- Photolysis: when 5 mg/L in methanol was irradiated by sunlight simulator more than 95% disappears within 48 h while a similar experiment with highly purified methanol solution reveals only very slow photolysis within the same period of irradiation and results were same with 10 mg/L in methanol solution (Crosby & Moilanen 1973; quoted, Choudhary & Hutzinger 1982);
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with \( NO_3 \) radical and \( k_{O3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference: \( k_{OH} = (6.6-16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0-2.3 d using a 12-h average daytime OH radical concn of \( 1.5 \times 10^6 \text{ molecule cm}^{-3} \) (Atkinson 1991)
- \( k_{OH} \) (calc) = \( 2.6-3.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) and the calculated tropospheric lifetime was 4.0-5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:
- Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:
- Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0-2.3 d (Atkinson 1991);
- tropospheric lifetime was calculated to be 4.0-5.5 d for dichloro-CDFs, for the reaction with OH radicals (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:
Soil:
Biota: mean biological t_{1/2} ~ 11 d in rainbow trout (Niimi 1986).

### TABLE 9.1.6.1
Reported aqueous solubilities and vapor pressures of 2,8-dichlorodibenzofuran at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aqueous solubility</strong></td>
<td><strong>Vapor pressure</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Rordorf 1989</strong></td>
</tr>
<tr>
<td></td>
<td><strong>generator column-GC/ECD</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>4.5</td>
<td>0.00384</td>
</tr>
<tr>
<td>25</td>
<td>0.0145</td>
</tr>
<tr>
<td>39.5</td>
<td>0.0339</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>ΔH_{sol}/(kJ mol⁻¹)</td>
<td>4–32°C</td>
</tr>
<tr>
<td>S/(mol/L) = a·exp[b·(t/°C)]</td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>1.24×10⁻²</td>
</tr>
<tr>
<td>b</td>
<td>0.062</td>
</tr>
<tr>
<td>ΔH_{sub}/(kJ mol⁻¹)</td>
<td>= 74.2</td>
</tr>
<tr>
<td>ΔH_{fus}/(kJ mol⁻¹)</td>
<td>= 101.423</td>
</tr>
<tr>
<td>ΔS_{fus}/(J mol⁻¹ K⁻¹)</td>
<td>= 55</td>
</tr>
</tbody>
</table>

**FIGURE 9.1.6.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,8-dichlorodibenzofuran.
9.1.1.7 3,6-Dichlorodibenzofuran

Common Name: 3,6-Dichlorodibenzofuran
Synonym: 3,6-DCDF
Chemical Name: 3,6-dichlorodibenzofuran
CAS Registry No: 94570-83-9
Molecular Formula: C₆H₃ClOC₆H₃Cl
Molecular Weight: 237.082

Melting Point (°C):
188  (Rordorf 1989)

Boiling Point (°C):
357  (Rordorf 1989)

Density (g/cm³):

Molar Volume (cm³/mol):
218.5  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
70.7  (Rordorf 1989)

Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
110.87  (Rordorf 1989)

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
38.1  (Rordorf 1989)

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
83  (Rordorf 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0252 (mp at 188°C)

Water Solubility (g/m³ or mg/L at 25°C):
1.76  (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
0.684; 1.76  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.0 × 10⁻⁴, 6.3 × 10⁻³, 0.12, 1.60, 15 (25, 50, 75, 100, 125°C, gas saturation-GC, Rordorf 1985a,b, 1987, 1989)
0.0355  (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
0.0123; 0.0355 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
log (Pₜ/mmHg) = 39.18 – 5755/(T/K) – 9.466·log (T/K) (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C):
4.57  (calculated-SOFA model, Govers & Krop 1998)
4.68; 4.57  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log $K_{ow}$:
5.08  (calculated-SOFA model, Govers & Krop 1998)
5.44; 5.08  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF or log $K_b$:
4.81  (lipid wt. basis, calculated-SOFA model, Govers & Krop 1998)
5.05; 4.81  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, log $K_{OC}$:

5.35  (sediment/water, calculated-SOFA model, Govers & Krop 1998)
5.18; 5.35  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, data at other temperatures see reference:

$k_{OH} = (6.6–16) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)

$k_{OH(calc)} = (2.6–3.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: mean biological $t_{1/2} = 24$ d in rainbow trout (Niimi & Oliver 1986)
9.1.1.8 2,3,8-Trichlorodibenzofuran

Common Name: 2,3,8-Trichlorodibenzofuran
Synonym: 2,3,8-TCDF
Chemical Name: 2,3,8-trichlorodibenzofuran
CAS Registry No: 57117-32-5
Molecular Formula: C\(_{12}\)H\(_5\)Cl\(_3\)O, C\(_6\)H\(_3\)ClOC\(_6\)H\(_2\)Cl\(_2\)
Molecular Weight: 271.527

Melting Point (°C):
189–191 (Rordorf 1989)

Boiling Point (°C):
408.4 (Rordorf 1989)

Density (g/cm\(^3\)):

Molar Volume (cm\(^3\)/mol):
239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
70.8 (Rordorf 1989)

Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
111.823 (Rordorf 1989)

Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
30.9 (Rordorf 1989)

Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
67 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming \(\Delta S_{ fus} = 56\) J/mol K), F:

Water Solubility (g/m\(^3\) or mg/L at 25°C):
0.291 (supercooled liquid \(S_L\), calculated-SOFA model, Govers & Krop 1998)
0.113, 0.291 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.0 \times 10^{-5}, 9.9 \times 10^{-4}, 2.0 \times 10^{-2}, 0.26, 2.50 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
4.27 \times 10^{-3} (supercooled liquid \(P_L\), calculated-SOFA model, Govers & Krop 1998)
2.48 \times 10^{-4} (solid \(P_S\), gas saturation-GC/MS, Mader & Pankow 2003)
0.0108 (supercooled liquid \(P_L\), calculated from \(P_S\) assuming \(\Delta S_{ fus} = 56\) J/mol K, Mader & Pankow 2003)

log (\(P_L/mmHg\)) = 37.66 – 5911/(T/K) – 8.932·log (T/K) (supercooled liquid \(P_L\), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
3.24 (calculated-SOFA model, Govers & Krop 1998)
2.57; 3.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log \(K_{ow}\):
5.76 (calculated-SOFA model, Govers & Krop 1998)
5.75; 5.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Chlorinated Dibenzofurans

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):

- 4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.20; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, \( \log K_{OC} \):

- 6.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 6.26; 6.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

- Volatilization:
- Photolysis:
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with \( NO_3 \) radical and \( k_{O3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference:
  - \( k_{OH} = (3.4–12) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of 1.5 \( \times 10^6 \) molecule cm\(^{-3}\) (Atkinson 1991)
  - \( k_{OH(calc)} = (1.5–2.6) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

- Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991); calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
9.1.1.9 2,4,6-Trichlorodibenzofuran

Common Name: 2,4,6-Trichlorodibenzofuran
Synonym: 2,4,6-PCDF
Chemical Name: 2,4,6-trichlorodibenzofuran
CAS Registry No: 58802-14-6
Molecular Formula: C_{12}H_{5}Cl_{3}O, C_{6}H_{3}ClOC_{6}H_{2}Cl_{2}
Molecular Weight: 271.527

Melting Point (°C): 116–117 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C): 408.4 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆H_v (kJ/mol):
84.2 (Rordorf 1989)
Enthalpy of Sublimation, ∆H_subl (kJ/mol):
116.061 (Rordorf 1989)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
30.9 (Rordorf 1989)
Entropy of Fusion, ∆S_fus (J/mol K):
79 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.461 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.175; 0.461 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.33 × 10⁻⁴ (estimated, Van den Berg & Olie 1985)
8.2 × 10⁻⁵, 3.1 × 10⁻³, 6.8 × 10⁻², 1.0, 10.0 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
4.27 × 10⁻³ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
1.32 × 10⁻³, 4.27 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
9.22 × 10⁻⁴ (solid P_s, gas saturation-GC/MS, Mader & Pankow 2003)
7.50 × 10⁻³ (supercooled liquid P_L, calculated from P_s assuming ∆S_fus = 56 J/mol K, Mader & Pankow 2003)
log (P/L/mmHg) = 37.77 – 5908/(T/K) – 8.932·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
ln (P/Pa) = 37.264 – 13912/(T/K), temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
ln (P/Pa) = (35.837 ± 0.729) – (13090 ± 259)/(T/K); temp range 338–373 K (Knudsen effusion technique, Li et al. 2004)

Henry’s Law Constant (Pa·m³/mol at 25°C):
2.40 (calculated-SOFA model, Govers & Krop 1998)
2.82; 2.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{ow}:
5.64 (calculated-SOFA model, Govers & Krop 1998)
5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.99 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.18; 4.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Vaporization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3, or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (3.4 - 4.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (3.4 - 12) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 1.3–4.5 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a tri-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(calc) = (1.5 - 2.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime of 4.0–5.5 d for a tri-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991); calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical for a tri-chlorinated dibenzofuran (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:

![FIGURE 9.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorodibenzo]
9.1.1.10  2,4,8-Trichlorodibenzofuran

Common Name: 2,4,8-Trichlorodibenzofuran
Synonym: 2,4,8-TCDF
Chemical Name: 2,4,8-trichlorodibenzofuran
CAS Registry No: 54589-71-8
Molecular Formula: C_{12}H_{5}Cl_{3}O, C_{6}H_{3}ClOC_{6}H_{2}Cl_{2}
Molecular Weight: 271.527
Melting Point (°C):
155–156 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
392.5 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
239.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
78.7 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
112.3 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
32.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
76 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0542 (mp at 154°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.494 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.157; 0.494 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9.1 × 10⁻⁶* (gas saturation-GC, Rordorf 1989)
5.75 × 10⁻³ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
log (P_L/mmHg) = 37.78 – 5809/(T/K) – 8.932·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
1.38 × 10⁻³, 5.75 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
3.09 (calculated-SOFA model, Govers & Krop 1998)
2.88; 3.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Water Partition Coefficient, log K_{OW}:
5.64 (calculated-SOFA model, Govers & Krop 1998)
5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{B}:
4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.18; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Chlorinated Dibenzofurans

Sorption Partition Coefficient, log $K_{OC}$:
6.06; 6.14 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
\[
k_{OH} = (3.4–12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule cm}^{-3} \text{ (Atkinson 1991)}
\]
\[
k_{OH}(calc) = (1.5–2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)}
\]
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);
calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:
Ground water:
Sediment:
Soil:
Biota:

### TABLE 9.1.10.1
Reported vapor pressures of 2,4,8-tetrachlorodibenzofuran at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P/\text{Pa}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>$9.1 \times 10^{-5}$</td>
</tr>
<tr>
<td>50</td>
<td>$3.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>75</td>
<td>$6.1 \times 10^{-2}$</td>
</tr>
<tr>
<td>100</td>
<td>0.82</td>
</tr>
<tr>
<td>125</td>
<td>8.0</td>
</tr>
</tbody>
</table>

$\Delta H_f/(\text{kJ mol}^{-1}) = 78.7$
$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 112.3$
$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 32.6$
$\Delta S_{fus}/(\text{J mol}^{-1} \text{ K}^{-1}) = 76$
FIGURE 9.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,8-trichlorodibenzofuran.
9.1.1.11  1,2,3,4-Tetrachlorodibenzofuran

Common Name: 1,2,3,4-Tetrachlorodibenzofuran
Synonym: 1,2,3,4-TCDF
Chemical Name: 1,2,3,4-tetrachlorodibenzofuran
CAS Registry No: 24478-72-6
Molecular Formula: C_{12}H_{4}Cl_{4}O, C_{6}H_{2}Cl_{2}OC_{6}H_{2}Cl_{2}
Molecular Weight: 305.978
Melting Point (°C):  
168.5–169  (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):  
438.3  (Rordorf 1989)
Density (g/cm³):  
(calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):  
260.3  (Rordorf 1989)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):  
84.4  (Rordorf 1989)
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):  
122.826  (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):  
36.6  (Rordorf 1989)
Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):  
83  (Rordorf 1989)
Fugacity Ratio at 25°C (assuming $\Delta S_{ fus} = 56$ J/mol K), $F$:  
Water Solubility (g/m³ or mg/L at 25°C):  
0.0717  (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
0.0306; 0.0717  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
$4.1 \times 10^{-6}, 1.9 \times 10^{-4}, 5.1 \times 10^{-3}, 8.7 \times 10^{-2}, 1.0$  (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
6.76 $\times 10^{-4}$ (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
log ($P_L$/mmHg) = 36.02 – 6019/(T/K) – 8.399·log (T/K)  (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):  
2.75  (calculated-SOFA model, Govers & Krop 1998)
1.74; 2.75  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log $K_{ ow}$:  
6.17  (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
6.34  (calculated-SOFA model, Govers & Krop 1998)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:
- 4.92 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.22; 4.92 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:
- 7.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 7.18; 7.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis half-life, $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH} = (1.4–8.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
- $k_{OH}(calc) = (0.8–1.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 154, 134$ L kg$^{-1}$ d$^{-1}$; $k_2 >1.8, >1.4$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 171$ L kg$^{-1}$ d$^{-1}$, 220 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: half-lives in gold fish: $t_{1/2} < 0.4$ d for PBO treated and $t_{1/2} > 0.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.12  1,2,3,7-Tetrachlorodibenzofuran

Common Name: 1,2,3,7-Tetrachlorodibenzofuran
Synonym: 1,2,3,7-TCDF
Chemical Name: 1,2,3,7-tetrachlorodibenzofuran
CAS Registry No: 83704-22-7
Molecular Formula: C_{12}H_4Cl_4O, C_6H_2Cl_2OC_6H_2Cl_2
Molecular Weight: 305.978
Melting Point (°C):
  167.5–168  (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
  438.3  (Rordorf 1989)
Density (g/cm³):
  260.3  (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
  260.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆H_v (kJ/mol):
  84.4  (Rordorf 1989)
Enthalpy of Sublimation, ∆H_sub (kJ/mol):
  122.879  (Rordorf 1989)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
  36.6  (Rordorf 1989)
Entropy of Fusion, ∆S_fus (J/mol K):
  83  (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  0.0805  (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
  0.0306; 0.0805  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  4.2 × 10⁻⁶, 1.9 × 10⁻⁴, 5.2 × 10⁻³, 8.9 × 10⁻², 1.1  (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation
    method, Rordorf 1989)
  7.08 × 10⁻⁴ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
  1.41 × 10⁻⁴, 7.08 × 10⁻⁴  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
  log (P_L/mmHg) = 36.07 – 6015/(T/K) – 8.399·log (T/K)  (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI
    correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  2.57  (calculated-SOFA model, Govers & Krop 1998)
  1.78; 2.57  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log K_{ow}:
  6.31  (calculated-SOFA model, Govers & Krop 1998)
  6.04; 6.31  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{bi}:
  3.41  (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
  4.93  (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
  5.23; 4.93  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, log $K_{OC}$:

- 7.07 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 7.10; 7.07 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Volutilization:**
Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)

**Oxidation:** rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, as indicated, *data at other temperatures see reference:
- $k_{OH}(calc) = (4.9 – 6.0) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (1.4 – 8.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime $\tau = 1.9–11$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)
- $k_{OH}(calc) = (0.8 – 1.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime $\tau = 7.7–18$ d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 142$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.007$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 171$ L kg$^{-1}$ d$^{-1}$, 220 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

**Air:** using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

**Surface water:**

**Ground water:**

**Sediment:** degradation $t_{1/2} = 20–200$ yr for all homologues (Suzuki et al. 2000)

**Soil:**

**Biota:** $t_{1/2} = 96$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.13 1,2,7,8-Tetrachlorodibenzofuran

Common Name: 1,2,7,8-Tetrachlorodibenzofuran
Synonym: 
Chemical Name: 1,2,7,8-tetrachlorodibenzofuran
CAS Registry No: 58802-20-3
Molecular Formula: C_{12}H_4Cl_4O, C_6H_2Cl_2OC_6H_2Cl_2
Molecular Weight: 305.978
Melting Point (°C): 210–211 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C): 438.3 (Rordorf 1989)
Density (g/cm³): 
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ f fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
Octanol/Air Partition Coefficient, $\log K_{OA}$:

- Bioconcentration Factor, log BCF or $\log K_{B}$:
  - 4.97 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
  - 5.22; 4.97 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.20 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constant, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
- Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis half-life, $t_{1/2} = 35$ h with PCDF dispersed as solid films (Buser 1988);
- $k = 0.014$ min$^{-1}$ with $t_{1/2} = 50$ min in pure water and $k = 0.0041$ min$^{-1}$ with $t_{1/2} = 170$ min in 60% acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor; $k = 0.08$ h$^{-1}$ with $t_{1/2} = 8.3$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH} = (1.4–8.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
- $k_{OH(calc)} = (0.8–1.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 162, 130$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.14, >1.0$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 171$ L kg$^{-1}$ d$^{-1}$, 220 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:
- Ground water:
- Sediment: degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:
- Biota: $t_{1/2} = 4.9$ d for PBO treated goldfish, and $t_{1/2} < 0.7$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.14 1,3,6,8-Tetrachlorodibenzofuran

Common Name: 1,3,6,8-Tetrachlorodibenzofuran
Synonym:
Chemical Name: 1,3,6,8-tetrachlorodibenzofuran
CAS Registry No: 71998-72-6
Molecular Formula: C_{12}H_4Cl_4O, C_6H_2Cl_2OC_6H_2Cl_2
Molecular Weight: 305.978
Melting Point (°C):
177–178 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
438.3 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
83.8 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
122.36 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
36.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
81 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.212 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
0.0625; 0.212 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.6 × 10^{-6}, 1.6 × 10^{-4}, 4.3 × 10^{-3}, 7.4 × 10^{-2}, 0.88 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
1.17 × 10^{-3} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
log (P_L/mmHg) = 36.34 – 6020/(T/K) – 8.399·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
2.95 × 10^{-4}, 1.17 × 10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1.62 (calculated-SOFA model, Govers & Krop 1998)
2.04; 1.62 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log K_{ow}:
6.37 (shake flask/slow stirring-GC/MS, fly-ash extract, Sijm et al. 1989)
6.06 (calculated-SOFA model, Govers & Krop 1998)
5.92; 6.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log $K_B$:
- 5.0 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.23; 5.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:
- 6.71 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 6.76; 6.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (1.4–8.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
  - $k_{OH}(calc) = (0.8–1.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
- Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radicals (Kwok et al. 1995).
- Surface water:
- Ground water:
- Sediment: degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (Suzuki et al. 2000)
- Soil:
- Biota:
### 1,3,7,8-Tetrachlorodibenzofuran

**Common Name:** 1,3,7,8-Tetrachlorodibenzofuran  
**Synonym:** 1,3,7,8-TCDF  
**Chemical Name:** 1,3,7,9-tetrachlorodibenzofuran  
**CAS Registry No:** 57117-35-8  
**Molecular Formula:** \( C_{12}H_4Cl_4O \), \( C_6H_2Cl_2OC_6H_2Cl_2 \)  
**Molecular Weight:** 306  
**Melting Point (°C):**  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 260.3 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):**  
**Enthalpy of Sublimation, \( \Delta H_{sub} \) (kJ/mol):**  
**Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):**  
**Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \) J/mol K), F:**  
**Water Solubility (g/m³ or mg/L at 25°C):** 0.116 (supercooled liquid \( S_L \), calculated-SOFA model, Govers & Krop 1998) 0.0463; 0.116 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)  
**Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):** 6.03 × 10⁻⁴ (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998) 2.00 × 10⁻⁴, 6.03 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003) 3.51 × 10⁻⁵ (solid \( P_S \), gas saturation-GC/MS, Mader & Pankow 2003) \[ \log (P_L/mmHg) = 36.20 - 6020/(T/K) - 8.399 \times \log (T/K) \] (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):** 1.55 (calculated-SOFA model, Govers & Krop 1998) 1.91; 1.55 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)  
**Octanol/Air Partition Coefficient, log \( K_{oa} \):**  
**Bioconcentration Factor, log BCF or log \( K_B \):** 3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993) 5.01 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998) 5.23; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)  
Environmental Fate Rate Constants, k, and Half-Lives, t<sub>½</sub>:

Volatileization:

Oxidation: rate constant k for gas-phase second order rate constants, k<sub>OH</sub> for reaction with OH radical, k<sub>No3</sub> with NO<sub>3</sub> radical and k<sub>O3</sub> with O<sub>3</sub> or as indicated, *data at other temperatures see reference:

k<sub>OH(calc)</sub> = (4.9 – 6.0) × 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>–1</sup> s<sup>–1</sup> at room temp. (Atkinson 1991)

k<sub>OH</sub> = (1.4 – 8.3) × 10<sup>–12</sup> cm<sup>3</sup> molecule<sup>–1</sup> s<sup>–1</sup> with calculated tropospheric lifetime τ = 1.9–11 d, using a 12-h average daytime OH radical concn of 1.5 × 10<sup>6</sup> molecule/cm<sup>3</sup> for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

k<sub>OH(calc)</sub> = (0.8 – 1.9) × 10<sup>–12</sup> cm<sup>3</sup> molecule<sup>–1</sup> s<sup>–1</sup> with a calculated lifetime τ = 7.7–18 d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k<sub>i</sub> and k<sub>2</sub>):

k<sub>i</sub> = 164, 293 L kg<sup>–1</sup> d<sup>–1</sup>; k<sub>2</sub> < 0.1, > 1.4 d<sup>–1</sup> (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

k<sub>i</sub> = 171 L kg<sup>–1</sup> d<sup>–1</sup>, 220 L kg<sup>–1</sup> d<sup>–1</sup> (average k<sub>i</sub> for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5 × 10<sup>6</sup> molecule/cm<sup>3</sup>, the tropospheric lifetime of a tetra-CDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: degradation t<sub>½</sub> = 20–200 yr for all homologues (Suzuki et al. 2000)

Soil:

Biota: t<sub>½</sub> >7 d for PBO treated goldfish and t<sub>½</sub> < 0.5 d for control fish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.16 1,3,7,9-Tetrachlorodibenzofuran

Common Name: 1,3,7,9-Tetrachlorodibenzofuran
Synonym: 1,3,7,9-TCDF
Chemical Name: 1,3,7,9-tetrachlorodibenzofuran
CAS Registry No: 64560-17-4
Molecular Formula: C_{12}H_{4}Cl_{4}O, C_{6}H_{2}Cl_{2}OC_{6}H_{2}Cl_{2}
Molecular Weight: 305.978
Melting Point (°C):
  206.5–207.5 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C):
  438.3 (calculated, Rordorf 1989)
Density (g/cm³):
  260.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
  83.3 (Rordorf 1989)
Enthalpy of Sublimation, \( \Delta H_{sub} \) (kJ/mol):
  121.988 (Rordorf 1989)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
  36.6 (Rordorf 1989)
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
  80 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \) J/mol K), \( F \):
Water Solubility (g/m³ or mg/L at 25°C):
  0.104 (supercooled liquid \( S_L \), calculated-SOFA model, Govers & Krop 1998)
  0.0422; 0.104 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  2.5 \times 10^{-6}, 1.1 \times 10^{-4}, 2.7 \times 10^{-3}, 4.5 \times 10^{-2}, 0.51 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
  4.37 \times 10^{-4} (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998)
  1.78 \times 10^{-4}, 4.36 \times 10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
  \log (P_L/mmHg) = 36.15 – 6018/(T/K) – 8.399\log (T/K) (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  1.26 (calculated-SOFA model, Govers & Krop 1998)
  1.86; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log \( K_{OW} \):
  6.39 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
  6.22 (calculated-SOFA model, Govers & Krop 1998)
  6.00; 6.22 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log \( K_{OA} \):
Bioconcentration Factor, log \( BCF \) or log \( K_{pL} \):
  3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
  5.06 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
  5.23; 5.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Sorption Partition Coefficient, log $K_{OC}$:
- 6.91 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 7.00; 6.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}\text{(calc)} = 8.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (1.4–8.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ (Atkinson 1991)
- $k_{OH}\text{(calc)} = (0.8–1.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 164, 293$ L kg$^{-1}$ d$^{-1}$; $k_2 < 0.1, >1.4$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 171$ L kg$^{-1}$ d$^{-1}$, 220 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: degradation $t_{1/2} = 20–200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} >7$ d for PBO treated gold fish and $t_{1/2} < 0.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.17  2,3,7,8-Tetrachlorodibenzofuran

![Chemical Structure](image_url)

**Common Name:** 2,3,7,8-Tetrachlorodibenzofuran  
**Synonym:** 2,3,7,8-TCDF  
**Chemical Name:** 2,3,7,8-Tetrachlorodibenzofuran  
**CAS Registry No:** 51207-31-9  
**Molecular Formula:** $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$  
**Molecular Weight:** 305.978

**Melting Point (°C):**  
227 (Lide 2003)

**Boiling Point (°C):**  
438.3 (calculated, Rordorf 1989)

**Density (g/cm³ at 20°C):**  
260.3 (calculated-Le Bas method at normal boiling point)  
199.4 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

**Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):**  
80.3 (Rordorf 1989)

**Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):**  
119.699 (Rordorf 1989)

**Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):**  
36.6 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

**Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):**  
73.2 (Rordorf 1989; quoted, Passivirta et al. 1999)

**Fugacity Ratio at 25°C, F:**  
0.0104 (calculated-assuming $\Delta S_{fus} = 56$ J/mol K and mp = 227°C)  
0.00256 (calculated- $\Delta S_{fus}$ and mp, Passivirta et al. 1999)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):**  
$4.19 \times 10^{-4}$ (22.7°C, generator column-HPLC/LSC, Friesen et al. 1990)  
$3.51 \times 10^{-3}$ (calculated-QSAR, Fiedler & Schramm 1990)  
$4.20 \times 10^{-4}; 5.32 \times 10^{-4}$ (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
$0.0413; 0.0413$ (supercooled liquid $S_L$, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)  
$log [S_L/(mol/L)] = 0.655 – 1915/(T/K)$, (supercooled liquid, Passivirta et al. 1999)  
$0.0243; 0.0413$ (GC-R1 correlation; calculated-SOFA method, Wang & Wong 2003)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
$2.0 \times 10^{-6}$ (quoted, Van den Berg & Olie 1985)  
$2.0 \times 10^{-6}, 8.5 \times 10^{-5}, 2.1 \times 10^{-3}, 3.3 \times 10^{-2}, 0.38$ (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)  
$1.23 \times 10^{-4}$ (GC-RT correlation, supercooled liquid $P_L$, Eitzer & Hites 1988, 1991; quoted, Della Site 1997)  
$1.13 \times 10^{-4}$ (GC-RT correlation, supercooled liquid $P_L$, Eitzer & Hites 1989; quoted, Della Site 1997)  
$2.00 \times 10^{-4}$ (supercooled liquid $P_L$, Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)  
$1.23 \times 10^{-4}, 1.13 \times 10^{-4}$ (calculated from reported $P_L$, solid vapor pressures, Della Site 1997)  
$7.50 \times 10^{-4}$ (corrected supercooled liquid $P_L$ in Eitzer & Hites 1988, Eitzer & Hites 1998)  
$1.62 \times 10^{-4}; 3.72 \times 10^{-4}$ (supercooled liquid $P_L$, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)  
$7.39 \times 10^{-4}; 1.89 \times 10^{-6}$ (supercooled liquid $P_L$ from GC-RT correlation; converted to solid $P_S$ with fugacity ratio F, Passivirta et al. 1999)  
$log (P_L/Pa) = 12.48 – 5425/(T/K)$ (solid, Passivirta et al. 1999)  
$log (P_L/Pa) = 8.66 – 3515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.678 × 10⁻⁵ (solid Pₜ, gas saturation-GC/MS, Mader & Pankow 2003)
1.718 × 10⁻³ (supercooled liquid Pₜ, calculated from Pₜ assuming ΔS_{fus} = 56 J/mol K, Mader & Pankow 2003)

log (P/μmHg) = 35.91 – 0.019(T/K) – 8.399·log (T/K) (supercooled liquid Pₜ, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
8.91 × 10⁻⁴, 3.72 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
1.50  (calculated for tetrachloro-PCDFs, Eitzer & Hites 1989)
1.70  (gas stripping-GC, 21°C, Friesen et al. 1993)
1.17; 2.69 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

log [H/(Pa m³/mol)] = 8.01 – 1598/(T/K) (Passivirta et al. 1999)
1.66; 2.69 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
5.82 (HPLC-RT correlation, Burkhard & Kuehl 1986)
6.53 (shake flask/slow stirring-GC/MS, from mixture of fly ash extract, Sijm et al. 1989)
6.19 (correlated, Ma et al. 1990)
7.10 (calculated-QSAR, Fiedler & Schramm 1990)
7.70 (calculated, Broman et al. 1991)
5.83 (HPLC-RT correlation, Jackson et al. 1993)
6.53 (recommended, Hansch et al. 1995)
6.46 (calculated-SOFA model, Govers & Krop 1998)
6.46, 6.58 (quoted, calculated-solubility log S_L and regression from lit. log K_{OW}, Passivirta et al. 1999)
6.225 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.42 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
10.02; 9.44 (generator column-GC/ECD; calculated, Harner et al. 2000)
10.90 (7°C, GC retention time correlation, Harner et al. 2000)
log K_{OA} = –4.92 + 4450/(T/K); temp range 10–50°C (Harner et al. 2000)

Bioconcentration Factor, log BCF:
4.82 (guppy, Opperhuizen et al. 1986)
3.78, 3.39 (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)
3.64, 3.41 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
3.82 (guppy, quoted, Opperhuizen & Sijm 1990)
4.19; 4.12 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.19; 4.33; 5.02 (guppies, 21-d exposure, lipid wt basis: measured-C_w/C_a; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 6.35 (fish with 5% lipid: wet weight basis, Geyer et al. 2000)
6.54, 5.75 (fish muscle log BCF, calculated from water, sediment, Wu et al. 2001)
5.22; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC}:
5.20 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
7.50 (calculated, Broman et al. 1991)
6.62 (calculated-K_{OC}, Kollig 1993)
5.18; 5.34 (sediment in lake mesocosm, Muir et al. 1992)
7.08; 7.29 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
7.32; 7.29 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

Volatilization:
Photolysis: sunlight induced photolysis \( t_{1/2} = 220 \) min in isooctane solution, and solid phase \( t_{1/2} = 120 \) h with PCDF dispersed as solid films (Buser 1988);
photolytic \( t_{1/2} = 9.8 \) h in extract of fly-ash and in tetradecane solution for native congener and \( t_{1/2} = 3.0 \) h for \(^{13}\text{C}-\)labelled congener (Tysklind & Rappe 1991).

Hydrolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:
\( k_{\text{OH}}(\text{calc}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Atkinson 1987b)
\( k_{\text{O}_3} = 1.32 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1} \) oxidative degradation rate constant for water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palaschek & Scholz 1987);
\( k_{\text{OH}}(\text{calc}) = (2.4 - 3.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Atkinson 1991)
\( k_{\text{OH}}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated lifetime \( \tau = 7.7 - 18 \) d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
\( k_1 = 400 \text{ d}^{-1} \); \( k_2 = 0.062 \text{ d}^{-1} \) (guppy, exposed to fly-ash extract, Opperhuizen et al. 1986)
\( k_1 = 1228, 6853 \text{ d}^{-1} \); \( k_2 = 0.28, 2.60 \text{ d}^{-1} \) (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)
\( k_1 = 56, 453 \text{ L kg}^{-1} \text{ d}^{-1} \); \( k_2 < 0.1, 0.22 \text{ d}^{-1} \) (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
\( k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1} \), 220 L kg\(^{-1}\) d\(^{-1}\) (average \( k_1 \) for P\(_4\)CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
\( k_2 = 0.0058 \text{ d}^{-1} \) with a biological \( t_{1/2} = 58 \) d (blue mussel, 99-d exposure, Hekeoten et al. 1994)
\( k_1 = 603 \text{ L kg}^{-1} \text{ d}^{-1} \); \( k_2 = 0.292 \text{ d}^{-1} \) (guppy, 21-d exposure, wet wt base, Loonen et al. 1994a)
\( k_1 = 0.0263 \text{ d}^{-1} \) with \( t_{1/2} = 26 \) d (newly contaminated oysters, Gardinali et al. 2004)
\( k_2 = 0.0194 \text{ d}^{-1} \) with \( t_{1/2} = 36 \) d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:
Air: using a 12-h average daytime OH radical concn of \( 1.5 \times 10^6 \) molecule cm\(^{-3}\), the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991);
calculated room temp. tropospheric lifetime to be 7.7–18 d for the gas-phase reaction with OH radical (Kwok et al. 1995);
\( t_{1/2} = 320 \) h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: \( t_{1/2} = 90 \) min in isooctane solution in summer sunlight (Palaschek & Scholz 1987);
suggested \( t_{1/2} = 6400 \) h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: \( t_{1/2} = 61 \) yr (Geyer et al. 2000)
degradation \( t_{1/2} = 20–200 \) yr in sediment for all homologues (Suzuki et al. 2000)
\( t_{1/2} = 550 \) 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: degradation \( t_{1/2} = 5–50 \) yr in soil (Suzuki et al. 2000)
\( t_{1/2} = 550 \) 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: Elimination \( t_{1/2} = 2 \) d from rat (Birnbaum et al. 1980; quoted, Birnbaum 1985);
\( t_{1/2} = 8 \) d from monkey (Birnbaum et al. 1981; quoted, Birnbaum 1985);
\( t_{1/2} = 2–4 \) d from mouse (Decad et al. 1981b; quoted, Birnbaum 1985);
\( t_{1/2} = 40 \) d from guinea pig (Decad et al. 1981a; Ioannou et al. 1983; quoted, Birnbaum 1985);
elimination half-lives: in guinea pigs, 20 d; rats, < 2 d; monkeys, 8 d; and mice, 2–4 d (quoted, Van den Berg & Olie 1985);
t_{1/2} < 336 d in carp (Kuehl et al. 1987);
elimination t_{1/2} = 3.0 d, 0.27 d (rainbow trout, exposed to 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988);
elimination t_{1/2} = 0.8 d for lactating cows (Olling et al. 1991);
$t_{1/2}$ >7 d for PBO treated goldfish, t_{1/2} = 3.1 d for control fish in 120-h exposure studies (Sijm et al. 1993)
 elimination t_{1/2} = 111 d from soft-shell clam (Brown 1994).
 biological t_{1/2} = 58 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
Depuration t_{1/2} = 26 d for newly contaminated oysters, and t_{1/2} = 36 d for chronically contaminated oysters
(Gardinial et al. 2004)
9.1.1.18 1,2,3,4,7-Pentachlorodibenzofuran

Common Name: 1,2,3,4,7-Pentachlorodibenzofuran
Synonym: 1,2,3,4,7-PCDF
Chemical Name: 1,2,3,4,7-pentachlorodibenzofuran
CAS Registry No: 83704-48-7
Molecular Formula: C\textsubscript{12}H\textsubscript{3}Cl\textsubscript{5}O, C\textsubscript{6}Cl\textsubscript{4}OC\textsubscript{6}H\textsubscript{3}Cl
Molecular Weight: 340.418
Melting Point (°C): 
Boiling Point (°C): 
Density (g/cm\textsuperscript{3}): 
Molar Volume (cm\textsuperscript{3}/mol): 281.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 
Enthalpy of Sublimation, \(\Delta H_{sub}\) (kJ/mol): 
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol): 
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K): 
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56 J/mol K\)), F: 

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C): 
0.0179 (supercooled liquid SL, calculated-SOFA model, Govers & Krop 1998) 
0.00745; 0.0179 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003) 

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations): 
2.43 \times 10^{-5} (supercooled liquid PL, GC-RT correlation, Eitzer & Hites 1989) 
2.09 \times 10^{-5} (supercooled liquid PL, calculated-SOFA model, Govers & Krop 1998) 
log (PL/mmHg) = 34.22 – 6088/(T/K) – 7.865\cdot log (T/K) (supercooled liquid PL, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003) 

Henry’s Law Constant (Pa\textsuperscript{-m\textsuperscript{3}}/mol): 
2.24 (calculated-SOFA model, Govers & Krop 1998) 
1.35; 2.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003) 

Octanol/Water Partition Coefficient, log K\textsubscript{OW}: 
6.53 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989) 
6.89 (calculated-SOFA model, Govers & Krop 1998) 
6.45; 6.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003) 

Octanol/Air Partition Coefficient, log K\textsubscript{OA}: 

Bioconcentration Factor, log BCF or log K\textsubscript{b}: 
4.80 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998) 
5.13; 4.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003) 

Sorption Partition Coefficient, log K\textsubscript{OC}: 
7.89 (sediment/water, calculated-SOFA model, Govers & Krop 1998) 
8.06; 7.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (3.6 – 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1991)}$

$k_{OH} = (1.0 – 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime } \tau = 3.6–15 \text{ d}, \text{ using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule/cm}^3 \text{ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)}$

$k_{OH}(calc) = (0.5 – 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated lifetime } \tau = 15–29 \text{ d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)}$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 68 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (goldfish after 120-h exposure: control fish, Sijm et al. 1993)}$

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (average } \text{k}_1 \text{ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)}$

$k_2 > 0.5, < 1.7 \text{ d}^{-1} \text{ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)}$

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991) calculated tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995)

Surface water:

Ground water:

Sediment:

Soil:

Biota: $t_{1/2} < 1.4 \text{ d for PBO treated goldfish and } t_{1/2} < 0.4 \text{ d for control fish in 120-h exposure studies (Sijm et al. 1993).}$
9.1.1.19 1,2,3,7,8-Pentachlorodibenzofuran

Common Name: 1,2,3,7,8-Pentachlorodibenzofuran
Synonym:
Chemical Name:
CAS Registry No: 57117-41-6
Molecular Formula: C_{12}H_{3}Cl_{5}O, C_{6}HCl_{3}OC_{6}H_{2}Cl_{2}
Molecular Weight: 340.418

Melting Point (°C):
225–227 (Rordorf 1989)

Boiling Point (°C):
464.7 (Rordorf 1989)

Density (g/cm³): 281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
83.6 (Rordorf 1989)

Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
128.978 (Rordorf 1989)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
42.4 (Rordorf 1989)

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
85 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), \( F \):

Water Solubility (g/m³ or mg/L at 25°C):
0.0108 (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998)

\[ \log \left( \frac{S_{L}/(mol/L)}{P_{L}/(Pa)} \right) = 0.794 – 2223/(T/K) \] (supercooled liquid, Passivirta et al. 1999)

0.0679; 0.0108 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.27 \times 10^{-3} (supercooled liquid \( P_L \), GC-RT correlation, Eitzer & Hites 1989)
2.3 \times 10^{-7}, 1.5 \times 10^{-5}, 4.0 \times 10^{-4}, 8.0 \times 10^{-3}, 0.11 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)

6.17 \times 10^{-3} (supercooled liquid \( P_L \), calculated-SOFA model, Govers & Krop 1998)

2.40 \times 10^{-4}; 2.35 \times 10^{-7} (supercooled liquid \( P_L \) from GC-RT correlation; converted to solid \( P_S \) with fugacity ratio \( F \), Passivirta et al. 1999)

\[ \log \left( \frac{P_S/(mmHg)}{P_L/(Pa)} \right) = 12.67 – 5750/(T/K) \] (solid, Passivirta et al. 1999)

\[ \log \left( \frac{P_L/(Pa)}{P_L/(mmHg)} \right) = 34.15 – 6081/(T/K) – 7.865 \times \log (T/K) \] (supercooled liquid \( P_L \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.70 \times 10^{-3}, 6.17 \times 10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry’s Law Constant (Pa·m³/mol or as indicated and reported temperature dependence equations):
1.91 (calculated-SOFA model, Govers & Krop 1998)

\[ \log \left( \frac{H/(Pa·m³/mol)}{P_L/(Pa)} \right) = 7.44 – 1306/(T/K) \] (Passivirta et al. 1999)

1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 6.79 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
- 6.99 (calculated-SOFA model, Govers & Krop 1998)
- 7.07 (estimated-solubility $S_i$ and regression eq. using lit. $K_{OW}$ values, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
- 11.4 (7°C, GC retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log $K_B$:
- 3.38 (guppy, Opperhuizen et al. 1986)
- 3.84, 3.61 (gold fish: treated with metabolic inhibitor PBO, control fish, 120-h exposure, Sijm et al. 1993)
- 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.12; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:
- 7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 8.03 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 8.11; 8.03 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:
- **Volatilization:**
  - Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution, $t_\text{1/2} = 10.0$ h for native congener (Tysklind & Rappe 1991)
  - Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:
    - $k_{OH}(\text{calc}) = 2.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
    - $k_{OH} = (1.0 - 4.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of 1.5 × 10$^6$ molecule cm$^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)
    - $k_{OH} = (0.5 - 1.0) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

- **Hydrolysis:**

- **Biodegradation:**

- **Biotransformation:**

- **Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):**
  - $k_1 = 98$, 252 L kg$^{-1}$ d$^{-1}$; $k_2 < 0.1$, < 0.1 d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
  - $k_1 = 110$ L kg$^{-1}$ d$^{-1}$, 174 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
  - $k_2 = 0.0126$ d$^{-1}$ with a biological $t_\text{1/2} = 24$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

- **Half-Lives in the Environment:**
  - Air: using a 12-h average daytime OH radical concn of 1.5 × 10$^6$ molecule cm$^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995); suggested $t_\text{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
  - Surface water: $t_\text{1/2} = 13200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
  - Ground water:
    - Sediment: $t_\text{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
    - Soil: $t_\text{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
    - Biota: elimination $t_\text{1/2} = 3.3–3.5$ d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989); $t_\text{1/2} > 7$ d for PBO treated goldfish and $t_\text{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993); biological $t_\text{1/2} = 24$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
9.1.1.20 1,2,4,7,8-Pentachlorodibenzoofuran

![Chemical structure of 1,2,4,7,8-Pentachlorodibenzoofuran](image)

Common Name: 1,2,4,7,8-Pentachlorodibenzoofuran
Synonym: 1,2,4,7,8-PeCDF
Chemical Name: 1,2,.4,7,8-pentachlorodibenzofuran
CAS Registry No: 83704-51-2
Molecular Formula: C₁₂H₃Cl₅O, C₆HCl₃OC₆H₂Cl₂
Molecular Weight: 340.418
Melting Point (°C): 236–238 (Rordorf 1989)
Boiling Point (°C): 464.7 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol): 281.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol): 85.2 (Rordorf 1989)
Enthalpy of Sublimation, ΔHₘₛₜ (kJ/mol): 128.442 (Rordorf 1989)
Enthalpy of Fusion, ΔH₉ₘₚ (kJ/mol): 42.4 (Rordorf 1989)
Entropy of Fusion, ΔS₉ₘₚ (J/mol K): 89 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS₉ₘₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00179 (supercooled liquid Sₐ, calculated-SOFa model, Govers & Krop 1998)
0.00618; 0.00179 (GC-RI correlation; calculated-SOFa method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.0 × 10⁻¹⁷, 1.1 × 10⁻⁵, 3.4 × 10⁻⁴, 6.7 × 10⁻³, 0.091 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
8.92 × 10⁻⁵ (supercooled liquid Pₐ, calculated-SOFa model, Govers & Krop 1998)
2.34 × 10⁻⁴, 8.91 × 10⁻⁵ (GC-RI correlation; calculated-SOFa method, Wang & Wong 2003)
log (Pₐ/mmHg) = 34.28 – 6082/(T/K) – 7.865·log (T/K) (supercooled liquid Pₐ, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1.62 (calculated-SOFa model, Govers & Krop 1998)
1.35; 1.91 (GC-RI correlation; calculated-SOFa method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log Kₐₐₜ:
6.26 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)
6.87 (calculated-SOFa model, Govers & Krop 1998)
6.40; 6.87 (GC-RI correlation; calculated-SOFa method, Wang & Wong 2003)
Octanol/Air Partition Coefficient, log Kₐₐₜ:
Bioconcentration Factor, log BCF or log $K_{bc}$:
- 3.02 (gold fish; treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
- 4.85 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.15; 4.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:
- 7.86 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 7.96; 7.86 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
  - Photolysis: $t_{1/2} = 48.5$ d on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
  - Oxidation: rate constant $k$ for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:
    - $k_{OH}(calc) = (1.8 – 1.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
    - $k_{OH} = (1.0 – 4.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)
    - $k_{OH}(calc) = (0.5 – 1.0) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)
- Hydrolysis:
  - Biodegradation:
  - Biotransformation:
  - Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
    - $k_1 = 63, 77$ L kg$^{-1}$ d$^{-1}$; $k_2 < 0.1, > 1.3$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
    - $k_1 = 110$ L kg$^{-1}$ d$^{-1}$, 174 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- Half-Lives in the Environment:
  - Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule cm$^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated tropospheric lifetime $\tau = 15–29$ d for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);
    - suggested $t_{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
  - Surface water: suggested $t_{1/2} = 13200$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000)
  - Ground water:
    - Sediment: suggested $t_{1/2} = 45000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
    - Soil: suggested $t_{1/2} = 45000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
    - Biota: elimination $t_{1/2} = 3.3–3.5$ d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);
      - $t_{1/2} > 7$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} < 1.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
Chlorinated Dibenzofurans

9.1.1.21 2,3,4,7,8-Pentachlorodibenzofuran

![Chemical Structure]

Common Name: 2,3,4,7,8-Pentachlorodibenzofuran
Synonym: 2,3,4,7,8-PCDF
Chemical Name: 2,3,4,7,8-pentachlorodibenzofuran
CAS Registry No: 57117-31-4
Molecular Formula: C_{12}H_{3}Cl_{5}O, C_{6}H_{2}Cl_{2}OC_{6}HCl_{3}
Molecular Weight: 340.418
Melting Point (°C):
196–196.5 (Kuroki et al. 1984, Rordorf 1989)
Boiling Point (°C):
464.7 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):

Enthalpy of Vaporization, ∆H_v (kJ/mol):
85.6 (Rordorf 1989)

Enthalpy of Sublimation, ∆H_{subl} (kJ/mol):
130.43 (Rordorf 1989)

Enthalpy of Fusion, ∆H_{ fus} (kJ/mol):
42.4 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ∆S_{ fus} (J/mol K):
90 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:
0.0208 (calculated-assuming ∆S_{ fus} = 56 J/mol K and mp = 196.5°C)
0.00196 (calculated-∆S_{ fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.000515 (calculated-QSAR, Fiedler & Schramm 1990)
0.000236 (22.7°C, generator column-GC/MS, Friesen et al. 1990)
0.00015 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0115; 7.11 × 10⁻³ (supercooled liquid S_L, quoted expl.; calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 1.076 – 2218/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.00481; 0.00711 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.17 × 10⁻³ (supercooled liquid P_L-GC-RT correlation, Eitzer & Hites 1988, 1991)
2.43 × 10⁻³ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
3.5 × 10⁻², 2.1 × 10⁻³, 6.7 × 10⁻⁴, 1.4 × 10⁻², 0.19 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
1.74 × 10⁻⁵ (supercooled liquid P_L, Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)
1.53 × 10⁻⁴ (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
1.95 × 10⁻⁵; 5.50 × 10⁻⁵ (supercooled liquid P_L, quoted expl.; calculated-SOFA model, Govers & Krop 1998)
1.91 × 10⁻⁴; 3.74 × 10⁻³ (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.62 – 5677/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.90 – 3462/(T/K) (supercooled liquid, Passivirta et al. 1999)
6.53 × 10^{-6} \text{ (solid P_s, gas saturation-GC/MS, Mader & Pankow 2003)}

3.20 \times 10^{-4} \text{ (supercooled liquid P_L, calculated from P_S assuming } \Delta S_{\text{ fus}} = 56 \text{ J/mol K, Mader & Pankow 2003)}

\log (P_s/\text{mmHg}) = 33.99 - 6084/(T/K) - 7.865 \log (T/K) \text{ (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)}

1.15 \times 10^{-4}, \ 5.50 \times 10^{-4} \text{ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)}

Henry’s Law Constant (Pa m^3/mol or as indicated and reported temperature dependence equations):

0.505 \text{ (calculated-P/C with selected values)}

0.575; 2.57 \text{ (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)}

\log (H/(Pa m^3/mol)) = 6.82 - 1244/(T/K) \text{ (Passivirta et al. 1999)}

1.29; 2.57 \text{ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)}

Octanol/Water Partition Coefficient, log K_{\text{OW}}:

6.92 \text{ (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)}

7.82 \text{ (calculated-QSAR, Fiedler & Schramm 1990)}

7.60 \text{ (calculated, Broman et al. 1991)}

6.92 \text{ (recommended, Hansch et al. 1995)}

7.11 \text{ (calculated-SOFA model, Govers & Krop 1998)}

7.11, 6.90 \text{ (quoted, calculated-solubility log S_L and regression from lit. log K_{\text{OW}}, Passivirta et al. 1999)}

6.757 \text{ (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)}

6.56; 7.11 \text{ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)}

Octanol/Air Partition Coefficient, log K_{\text{OA}} at 25°C or as indicated:

10.09 \text{ (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)}

11.52 \text{ (7°C, GC-retention time correlation, Harner et al. 2000)}

Bioconcentration Factor, log BCF:

3.70 \text{ (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)}

5.14; 4.92 \text{ (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)}

5.14; 5.15; 5.38 \text{ (guppies, 21-d exposure, lipid weight basis: measured-C_{\text{fish}}/C_{\text{w}}; calculated; rate constant ratio } k_1/k_2 \text{ from non-linear regression analysis, Loonen et al. 1994b)}

5.14; 4.79 \text{ (lipid wt basis, quoted exptl.; quoted exptl.; calculated-SOFA model, Govers & Krop 1998)}

5.62; 5.92, 6.92 \text{ (fish 5% lipid: wet wt basis; fish 10% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)}

6.42, 5.88 \text{ (fish muscle log BCF, calculated from water, sediment, Wu et al. 2001)}

5.08; 4.79 \text{ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)}

Bioaccumulation Factor, BAF:

1.44, 1.33 \text{ (rainbow trout, concn in food: 0.82, 9.01 ng/g, Muir et al. 1990)}

Sorption Partition Coefficient, log K_{\text{OC}}:

5.59 \text{ (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)}

7.40 \text{ (calculated, Broman et al. 1991)}

6.60, 6.92 \text{ (calculated-K_{\text{OC}}, Kollig 1993)}

8.20 \text{ (calculated-SOFA model, sediment/water, Govers & Krop 1998)}

8.30; 8.20 \text{ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)}

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: photolytic degradation t_{1/2} = 3.5 h of PCDD in extract of fly-ash in tetradeccane solution for native congener and t_{1/2} = 3.1 h for 13C-labelled congener (Tysklind & Rappe 1991)

Hydrolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with \( \text{NO}_3 \) radical and \( k_{\text{O}_3} \) with \( \text{O}_3 \) or as indicated, *data at other temperatures see reference:

\[
\begin{align*}
 k_{\text{OH}}(\text{calc}) &= (1.7\,\text{–}1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1991)} \\
 k_{\text{OH}} &= (1.0\,\text{–}4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime } \tau = 3.6\,\text{–}15 \text{d, using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule cm}^{-3} \text{ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)} \\
 k_{\text{OH}}(\text{calc}) &= (0.5\,\text{–}1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a calculated lifetime } \tau = 15\,\text{–}29 \text{d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)}
\end{align*}
\]

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_i \)) and Elimination (\( k_e \)) Rate Constants:

\[
\begin{align*}
 k_2 &= 0.0027 \text{ d}^{-1} \text{ (carp, calculated from data reported by Kuehl et al. 1987, Sijm et al. 1990)} \\
 k_1 &= 400 \text{ mL g}^{-1} \text{ d}^{-1}; k_2 = 0.079 \text{ d}^{-1} \text{ (guppy, Oppenhuizen et al. 1986)} \\
 k_2 &= 0.0064 \text{ d}^{-1} \text{ (liver of female rat, Van den Berg et al. 1989)} \\
 k_2 &= -2.1 \times 10^{-2}, 1.5 \times 10^{-2} \text{ d}^{-1} \text{ (rainbow trout, 2 to 21 d exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1990)} \\
 k_2 &= 10.1 \times 10^{-3} \text{ d}^{-1} \text{ and } k_2 = 8.10 \times 10^{-3} \text{ d}^{-1} \text{ and } k_2 = 12.6 \times 10^{-3} \text{ d}^{-1} \text{ and } k_2 = 11.4 \times 10^{-3} \text{ d}^{-1} \text{ (rainbow trout, 0–140 d and 0–180 d exposure at 0.82 ng/g PCDF concn.; 0–140 d and 0–180 d exposure at 9.01 ng/g PCDF concn., Muir et al. 1990)} \\
 k_1 &= 105, 561 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.11, < 0.1 \text{ d}^{-1} \text{ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)} \\
 k_1 &= 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (average } k_1 \text{ for } \text{P}_5\text{CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)} \\
 k_1 &= 0.0081 \text{ d}^{-1} \text{ with a biological } t_{\text{biol}} = 36 \text{ d (blue mussel, 99-d exposure, Hektoen et al. 1994)} \\
 k_1 &= 1012 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.044 \text{ d}^{-1} \text{ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)}
\end{align*}
\]

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of \( 1.5 \times 10^6 \text{ molecule cm}^{-3} \), the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be \( 3.6\,\text{–}15 \text{d} \) (Atkinson 1991); calculated room temp. tropospheric lifetime to be\( 15\,\text{–}29 \text{d} \) for the gas-phase reaction with OH radical (Kwok et al. 1995);

\( t_{\text{biol}} = 660 \text{ h at } 7^\circ\text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)} \).

Surface water: photolytic \( t_{\text{biol}} = 3.5 \text{ h} \) in the extract from fly-ash in tetradecane solution, for native congener and \( t_{\text{biol}} = 3.1 \text{ h} \) for \( ^{13}\text{C} \) labelled congener (Tysklind & Rappe 1991)

\( t_{\text{biol}} = 13200 \text{ h at } 7^\circ\text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)} \).

Groundwater:

Sediment: very persistent \( t_{\text{biol}} = 60 \text{ yr} \) (Geyer et al. 2000)

degradation \( t_{\text{biol}} = 20\,\text{–}200 \text{ yr} \) in sediment for all homologues (estimated, Suzuki et al. 2000);

\( t_{\text{biol}} = 550 000 \text{ h at } 7^\circ\text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)} \).

Soil: degradation \( t_{\text{biol}} = 5\,\text{–}50 \text{ yr} \) (estimated, Suzuki et al. 2000);

\( t_{\text{biol}} = 550 000 \text{ h at } 7^\circ\text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)} \).

Biota: elimination \( t_{\text{biol}} = 108 \text{ d in the liver of female rats (Van den Berg et al. 1989)} \);

\( t_{\text{biol}} = 69 \text{ d in rainbow trout at the 0.82 ng/g exposure concentration from 0–140 d data, } t_{\text{biol}} = 61 \text{ d at 9.0 ng/g exposure concentration from 0–180 d data; } t_{\text{biol}} = 65 \text{ d in whole body rainbow trout with 31-d dietary exposure (Muir et al. 1990)} \);

elimination \( t_{\text{biol}} = 48.5 \text{ d for lactating cows (Olling et al. 1991)} \);

\( t_{\text{biol}} = 6.1 \text{ d for PBO treated goldfish and } t_{\text{biol}} > 7 \text{ d for control fish in 120-h exposure studies (Sijm et al. 1993)} \)

biological \( t_{\text{biol}} = 49 \text{ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)} \)
9.1.1.22 1,2,3,4,6,8-Hexachlorodibenzofuran

Common Name: 1,2,3,4,6,8-Hexachlorodibenzofuran
Synonym: 1,2,3,4,6,8-HxCDF
Chemical Name: 1,2,3,4,6,8-Hexachlorodibenzofuran
CAS Registry No: 69698-60-8
Molecular Formula: C₁₂H₂Cl₆O, C₆H₂Cl₂OC₆Cl₄
Molecular Weight: 374.863
Melting Point (°C): 233.5–234 (Kuroki et al. 1984; Rordorf 1989)
Boiling Point (°C): 487.7 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, ∆HV (kJ/mol):
86 (Rordorf 1989)
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):
137.049 (Rordorf 1989)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)
Entropy of Fusion, ∆Sfus (J/mol K):
95 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F :
0.000332 (calculated- ∆Sfus and mp, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
6.08 × 10⁻³ (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 0.839 – 2520/(T /K), (supercooled liquid, Passivirta et al. 1999)
2.48 × 10⁻³, 5.08 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.9 × 10⁻⁸, 2.1 × 10⁻⁶, 8.1 × 10⁻⁵, 1.9 × 10⁻³, 0.031 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.67 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
1.74 × 10⁻⁵ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
9.39 × 10⁻³, 4.53 × 10⁻⁸ (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.84 – 6057/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.88 – 3540/(T/K) (supercooled liquid, Passivirta et al. 1999)
5.13 × 10⁻⁶, 1.74 × 10⁻⁵ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
log (P_L/mmHg) = 32.06 – 6015/(T/K) – 7.332·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa m³/mol at 25°C):
1.023 (calculated-SOFA model, Govers & Krop 1998)
log (H/(Pa m³/mol)) = 7.04 – 1020/(T/K) (Passivirta et al. 1999)
1.26; 1.012 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Chlorinated Dibenzofurans

Octanol/Water Partition Coefficient, log $K_{OW}$:

- 7.31 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 7.58 (calculated-solubility log $S_L$ and regression from lit. log $K_{OW}$s, Passivirta et al. 1999)
- 6.78; 7.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.96; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:


Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{1/2}$:

Volatilization:
Photolysis: $t_\text{1/2} = 59.8 \text{ h on spruce needle surfaces under sunlight irradiation}$ (Niu et al. 2003)

Hydrolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 168 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average $k_1$ for H$_6$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
suggested $t_\text{1/2} = 1400 \text{ h at } 7^\circ\text{C in Baltic Proper environment}$ (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_\text{1/2} = 28 \text{ 000 h at } 7^\circ\text{C in Baltic Proper environment}$ (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_\text{1/2} = 20–200 \text{ yr for all homologues}$ (estimated, Suzuki et al. 2000);
suggested $t_\text{1/2} = 450 \text{ 000 h at } 7^\circ\text{C in Baltic Proper environment}$ (Sinkkonen & Passivirta 2000).

Soil: degradation $t_\text{1/2} = 5–50 \text{ yr}$ (estimated, Suzuki et al. 2000);
suggested $t_\text{1/2} = 450 \text{ 000 h at } 7^\circ\text{C in Baltic Proper environment}$ (Sinkkonen & Passivirta 2000).

Biota: $t_\text{1/2} > 7 \text{ d for PBO treated goldfish in 120-h exposure studies}$ (Sijm et al. 1993)
9.1.1.23 1,2,3,4,7,8-Hexachlorodibenzofuran

Common Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
Synonym: 1,2,3,4,7,8-HxCDF
Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
CAS Registry No: 70658-26-9
Molecular Formula: C_{12}H_{2}Cl_{6}O, C_{6}H_{2}Cl_{2}OC_{6}Cl_{4}
Molecular Weight: 374.863

Melting Point (°C):
225.5–226.5 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point (°C):
487.7 (calculated, Rordorf 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ∆H_{v} (kJ/mol):
86.5 (Rordorf 1989)

Enthalpy of Sublimation, ∆H_{sub} (kJ/mol):
137.397 (Rordorf 1989)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
48.1 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ∆S_{fus} (J/mol K):
96 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:
0.0107 (calculated-assuming ∆S_{fus} = 56 J/mol K and mp = 226°C)
0.000402 (calculated- ∆S_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
8.25 × 10⁻⁶ (22.7°C, generator column-GC/MS, Friesen et al. 1990)
7.30 × 10⁻⁶ (computed-expert system SPARC, Kollig 1995)
8.2 × 10⁻⁶, 1.13 × 10⁻⁶ (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
8.01 × 10⁻⁴; 2.65 × 10⁻³ (supercooled liquid S_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 0.913 – 2516/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.64 × 10⁻¹, 2.65 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.093 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988; quoted, Della Site 1997)
3.2 × 10⁻¹, 2.4 × 10⁻⁶, 9.3 × 10⁻⁵, 2.2 × 10⁻³, 0.036 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.85 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)
8.90 × 10⁻⁸ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
3.09 × 10⁻⁶ (supercooled liquid P_L, Falconer & Bidleman 1994;)
8.67 × 10⁻⁸ (computed-expert system SPARC, Kollig 1995)
8.41 × 10⁻⁸, 3.68 × 10⁻⁸ (P_S solid vapor pressure calculated from reported P_L, Della Site 1997)

© 2006 by Taylor & Francis Group, LLC
Chlorinated Dibenzofurans

6.05 × 10⁻⁵ \( (\text{corrected supercooled liquid } P_L\text{, quoted exptl.; calculated-SOFA model, Govers & Krop 1998}) \)

5.62 × 10⁻⁶; 1.38 × 10⁻⁵ \( (\text{supercooled liquid } P_L, \text{ quoted exptl.; calculated-SOFA model, Govers & Krop 1998}) \)

2.87 × 10⁻⁸; 7.13 × 10⁻⁵ \( (\text{supercooled liquid } P_L \text{ from GC-RT correlation; converted to solid } P_S \text{ with fugacity ratio } F, \text{Passivirta et al. 1999}) \)

\[ \log (P_L/Pa) = 12.85 \text{ – } 6077/(T/K) \text{ (solid, Passivirta et al. 1999)} \]

\[ \log (P_L/Pa) = 7.81 \text{ – } 3564/(T/K) \text{ (supercooled liquid, Passivirta et al. 1999)} \]

\[ \log (P_L/\text{mmHg}) = 32.14 \text{ – } 6106/(T/K) \text{ – } 7.332 \log (T/K) \text{ (supercooled liquid } P_L, \text{ Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)} \]

3.24 × 10⁻⁶, 1.38 × 10⁻⁵ \( (\text{GC-RI correlation; calculated-SOFA method, } \text{Wang & Wong 2003}) \)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

1.454 \( (\text{calculated-P/C with selected values}) \)

4.26 \( (\text{computed-expert system SPARC, Kollig 1995}) \)

2.63; 1.91 \( (\text{quoted exptl.; calculated-SOFA model, Govers & Krop 1998}) \)

\[ \log [H/(Pa \text{ m³/mol})] = 6.90 \text{ – } 1048/(T/K) \text{ (Passivirta et al. 1999)} \]

1.26; 1.905 \( (\text{GC-RI correlation; calculated-SOFA method, } \text{Wang & Wong 2003}) \)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

7.70 \( (\text{calculated, Broman et al. 1991}) \)

7.86 \( (\text{computed-expert system SPARC, Kollig 1995}) \)

7.53 \( (\text{sediment/water, calculated-SOFA model, Govers & Krop 1998}) \)

7.54 \( (\text{calculated-solubility log } S_i \text{ and regression from lit. log } K_{OW}, \text{Passivirta et al. 1999}) \)

7.184 \( (\text{calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001}) \)

6.92; 7.53 \( (\text{GC-RI correlation; calculated-SOFA method, } \text{Wang & Wong 2003}) \)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated:

10.64 \( (\text{Finizio et al. 1997; quoted, Kaupp & McLachlan 1999}) \)

11.98 \( (7°C, \text{ GC-retention time correlation, Harner et al. 2000}) \)

Bioconcentration Factor, log \( BCF \):

4.91; 4.40 \( (\text{guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a}) \)

4.91; 4.99; 5.04 \( (\text{guppies, 21-d exposure, lipid weight basis: measured-C_{fish}/C_w; calculated; rate constant ratio } k_1/k_2 \text{ from non-linear regression analysis, Loonen et al. 1994b}) \)

4.57 \( (\text{lipid wt basis, calculated-SOFA model, Govers & Krop 1998}) \)

5.90, 5.26 \( (\text{fish muscle log } BCF_L, \text{ calculated from water, sediment, } \text{Wu et al. 2001}) \)

4.88; 4.57 \( (\text{GC-RI correlation; calculated-SOFA method, } \text{Wang & Wong 2003}) \)

Sorption Partition Coefficient, log \( K_{OC} \):

7.40 \( (\text{calculated, Broman et al. 1991}) \)

7.54 \( (\text{computed-expert system SPARC, Kollig 1995}) \)

8.83; 8.80 \( (\text{sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998}) \)

8.95; 8.80 \( (\text{GC-RI correlation; calculated-SOFA method, } \text{Wang & Wong 2003}) \)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis: photolytic \( t_{1/2} = 5.5 \text{ h of the PCDD in extract of fly ash in tetradecane solution for native congener} \) (Tysklind & Rappe 1991).

Hydrolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \text{ for reaction with OH radical, } k_{NO3} \text{ with NO}_3 \text{ radical and } k_{O3} \text{ with O}_3 \text{ or as indicated, *data at other temperatures see reference: } k_{O3}(aq.) = 7.28 \times 10^4 \text{ L·g}^{-1}·\text{min}^{-1}, \text{ oxidative degradation rate constant of water dissolved PDCF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)} \)
$k_{OH} = (0.7–2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a hexa-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 5.9–22 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

Biodegradation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

- $k_1 = 100, 439 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.31, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 = 0.0126 \text{ d}^{-1}$ with a biological $t_{1/2} = 24$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)
- $k_1 = 879 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.087 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
- $t_{1/2} = 1400 \text{ h at 7}^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Surface water: $t_{1/2} = 28 000 \text{ h at 7}^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Groundwater:

- Sediment: degradation $t_{1/2} = 20–200$ yr for all homologues (estimated, Suzuki et al. 2000);
- $t_{1/2} = 600 000 \text{ h at 7}^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Soil: degradation $t_{1/2} = 5–50$ yr (estimated, Suzuki et al. 2000);
- $t_{1/2} = 600 000 \text{ h at 7}^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).}$

Biota: $t_{1/2} \sim 336$ d in carp (Kuehl et al. 1987);
- elimination $t_{1/2} = 48.5 \text{ d from lactating cows (Olling et al. 1991);}$
- $t_{1/2} = 2.2 \text{ d for PBO treated goldfish and } t_{1/2} > 7 \text{ d for control fish in 120-h exposure studies (Sijm et al. 1993)}$
- biological $t_{1/2} = 24 \text{ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994).}$
Common Name: 1,2,3,6,7,8-Hexachlorodibenzofuran
Synonym:
Chemical Name: 1,2,3,6,7,8-hexachlorodibenzofuran
CAS Registry No: 57117-44-9
Molecular Formula: C_{12}H_2Cl_6O, C_6HCl_3OC_6HCl_3
Molecular Weight: 374.863
Melting Point (°C): 232–234 (Rordorf 1989)
Boiling Point (°C): 487.7 (calculated, Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔH_v (kJ/mol): 86.1 (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol): 137.083 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 48.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K): 95 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.000358 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.00226 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 0.125 – 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.56 × 10⁻³, 2.26 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7.33 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
2.9 × 10⁻⁸, 2.1 × 10⁻⁸, 8.2 × 10⁻⁸, 2.0 × 10⁻⁵, 0.031 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)
1.20 × 10⁻³ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
6.91 × 10⁻⁵; 2.47 × 10⁻⁴ (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)
log (P_s/Pa) = 12.87 – 6101/(T/K) (solid, Passivirta et al. 1999)
log (P_s/Pa) = 7.91 – 3954/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_s/mmHg) = 32.12 – 6108/(T/K) – 7.332·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
3.09 × 10⁻⁶, 1.20 × 10⁻⁵ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations:
1.91 (calculated-SOFA model, Govers & Krop 1998)
log (H/(Pa·m³/mol)) = 7.79 – 1439/(T/K), (Passivirta et al. 1999)
1.26; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:
7.60 (calculated, Broman et al. 1991)
7.57 (calculated-SOFA model, Govers & Krop 1998)
7.96 (estimated-solubility $S_i$ and regression eq. using lit. $K_{\text{OW}}$ values, Passivirta et al. 1999)
7.196 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated:
12.0 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_{\text{B}}$:
4.95; 4.49 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.95, 5.15; 5.24 (guppies, 21-d exposure, lipid weight basis: measured-$C_{\text{fish}}/C_{\text{w}}$; calculated; rate constant ratio $k_1/k_2$ from non-linear regression analysis, Loonen et al. 1994b)
4.58 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.51 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
4.87; 4.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:
7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
8.97; 8.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: photolytic $t_{1/2} = 5.9$ h in extract of fly-ash and in tetradecane solution for native congener (Tysklind & Rappe 1991);
$t_{1/2} = 74.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{\text{OH}}(\text{calc}) = (1.3 - 1.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
$k_{\text{OH}} = (0.7 - 2.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5 $\times$ 10$^6$ molecule/cm$^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
$k_1 = 103$, 460 L kg$^{-1}$ d$^{-1}$; $k_2 = 0.26$, < 0.1 d$^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 110$ L kg$^{-1}$ d$^{-1}$, 174 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_2$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
$k_2 = 0.0138$ d$^{-1}$ with a biological $t_{1/2} = 22$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)
$k_1 = 1310$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.078$ d$^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Ground water:
Sediment: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Biota: elimination $t_{1/2} = 73–156$ d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);
$t_{1/2} = 2.7$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)
biological $t_{1/2} = 22$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994).
9.1.1.25  1,2,3,7,8,9-Hexachlorodibenzofuran

Common Name: 1,2,3,7,8,9-Hexachlorodibenzofuran
Synonym: 1,2,3,7,8,9-HxCDF
Chemical Name: 1,2,3,7,8,9-hexachlorodibenzofuran
CAS Registry No: 72918-21-9
Molecular Formula: C₁₂H₂Cl₆O, C₆HCl₃OC₆HCl₃
Molecular Weight: 374.863
Melting Point (°C):
246–249 (Rordorf 1989)
230 (calculated, Passivirta et al. 1999)
Boiling Point (°C):
487.7 (calculated, Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Passivirta et al. 1999)
Enthalpy of Vaporization, ∆ Hv (kJ/mol):
Enthalpy of Sublimation, ∆ Hsubl (kJ/mol):
Enthalpy of Fusion, ∆ Hfus (kJ/mol):
Entropy of Fusion, ∆ Sfus (J/mol K):
96 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ∆ Sfus = 56 J/mol K), F:
0.00036 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.000859 (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 0.892 – 2526/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.06 × 10⁻³, 8.59 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.31 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)
2.24 × 10⁻⁶ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
4.01 × 10⁻³; 1.44 × 10⁻⁸ (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.91 – 6185/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.90 – 3625/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_L/mmHg) = 31.92 – 6114/(T/K) – 7.332·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
2.09 × 10⁻⁶, 2.24 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
0.955 (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa·m³/mol)] = 7.01 – 1136/(T/K) (Passivirta et al. 1999)
1.29; 0.955 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log K_{OW}:
7.00 (calculated, Broman et al. 1991)
7.76 (calculated-SOFA model, Govers & Krop 1998)
Chlorinated Dibenzofurans

7.57 (estimated-solubility S_L and regression eq. using lit. K_ow values, Passivirta et al. 1999)
7.125 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.07; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_OA at 25°C or as indicated:
12.17 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B:
4.71 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.04 (fish muscle log BCF_L calculated from water, Wu et al. 2001)
4.77; 4.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_OC:
9.08 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

Volatileization:
Photolysis: photolytic half-life in extract of fly-ash and in tetradeane solution: t_1/2 = 2.2 h for native congener and t_1/2 = 3.6 h for 13C-labelled congener (Tysklind & Rappe 1991);
t_1/2 = 78.8 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_OH for reaction with OH radical, k_NO3 with NO_3 radical and k_O3 with O_3 as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (1.5 – 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1991)}
k_{OH} = (0.7 – 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule/cm}^3 \text{ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)}

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 0.01651 \text{ d}^{-1} \text{ with a biological } t_1/2 = 18 \text{ d (blue mussel, 99-d exposure, Hektoen et al. 1994)}
k_2 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}; k_3 = 0.103 \text{ d}^{-1} \text{ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)}

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
t_1/2 = 1400 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Surface water: t_1/2 = 28000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Ground water:
Sediment: t_1/2 = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: t_1/2 = 500000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: biological t_1/2 = 18 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
9.1.1.26  1,2,4,6,7,8-Hexachlorodibenzofuran

Common Name: 1,2,4,6,7,8-Hexachlorodibenzofuran
Synonym: 1,2,4,6,7,8-HxCDF
Chemical Name: 1,2,4,6,7,8-hexachlorodibenzofuran
CAS Registry No: 67562-40-7
Molecular Formula: C_{12}H_2Cl_6O, C_6HCl_3OC_6HCl_3
Molecular Weight: 374.863
Melting Point (°C):
221–222  (Kuroki et al. 1986; Rordorf 1989; Passivirta et al. 1999)
Boiling Point (°C):
487.7  (calculated, Rordorf 1989)
Density (g/cm³):
302.1  (calculated-Le Bas method at normal boiling point)
225.2  (Passivirta et al. 1999)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
86.8  (Rordorf 1989)
Enthalpy of Sublimation, ΔH_{sub} (kJ/mol):
137.593  (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
48.1  (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
97  (Rordorf 1989; Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000483  (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
0.00451  (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)
log [S_L/(mol/L)] = 0.944 – 2512/(T/K), (supercooled liquid, Passivirta et al. 1999)
2.26 × 10^{-3}, 4.51 × 10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.5 × 10^{-8}, 2.6 × 10^{-6}, 1.0 × 10^{-4}, 2.4 × 10^{-3}, 0.040 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
1.35 × 10^{-5}  (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)
9.39 × 10^{-3}, 4.53 × 10^{-2} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.81 – 6006/(T/K), (solid, Passivirta et al. 1999)
log (P_L/Pa) = 7.74 – 3497/(T/K), (supercooled liquid, Passivirta et al. 1999)
log (P_L/mmHg) = 32.31 – 6108/(T/K) – 7.332·log (T/K) (supercooled liquid P_L, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
1.072  (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa·m³/mol)] = 6.80 – 985/(T/K), (Passivirta et al. 1999)
1.26; 1.072  (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Chlorinated Dibenzofurans

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 7.38 (calculated-SOFA model, Govers & Krop 1998)
- 7.51 (estimated-solubility $S_L$ and regression eq. using lit. $K_{ow}$ values, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF or log $K_b$:
- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.94; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{oc}$:
- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: $t_{1/2} = 58.2$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}$(calc) = 0.74 x 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (0.7 – 2.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 345, 293$ L kg$^{-1}$ d$^{-1}$; $k_2 < 0.10, > 2.4$ d$^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 170$ L kg$^{-1}$ d$^{-1}$, 369 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for H$_6$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_1 = 1101$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.103$ d$^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
- suggested $t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2} > 7$ d for PBO treated goldfish and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.27 1,2,4,6,8,9-Hexachlorodibenzofuran

Common Name: 1,2,4,6,8,9-Hexachlorodibenzofuran
Synonym: 1,2,3,4,8,9-HxCDF
Chemical Name: 1,2,4,6,8,9-hexachlorodibenzofuran
CAS Registry No: 69698-59-5
Molecular Formula: C_{12}H_{2}Cl_{6}O, C_{6}HCl_{3}OC_{6}HCl_{3}
Molecular Weight: 374.863
Melting Point (°C):
246–248 (Kuroki et al. 1984; Passivirta et al. 1999)
Boiling Point (°C):
487.7 (Rordorf 1989)
Density (g/cm³):
Molar Volume (cm³/mol):
302.1 (calculated-Le Bas method at normal boiling point)
225.2 (Passivirta et al. 1999)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
85.2 (Rordorf 1989)
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
136.462 (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
48.1 (Rordorf 1989)
Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):
93 (Rordorf 1989; Passivirta et al. 1999)
Fugacity Ratio at 25°C, $F$:
0.000245 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
0.00305 (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
$log [S_L/(mol/L)] = 0.892 – 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
1.92 × 10⁻³, 3.05 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.4 × 10⁻⁸, 1.7 × 10⁻⁶, 6.4 × 10⁻⁵, 1.5 × 10⁻³, 0.024 (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
9.22 × 10⁻⁶ (supercooled liquid $P_L$, GC-RT correlation, Eitzer & Hites 1989)
3.55 × 10⁻⁶ (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
7.69 × 10⁻⁵; 1.95 × 10⁻³ (supercooled liquid $P_L$ from GC-RT correlation; converted to solid $P_S$ with fugacity ratio $F$, Passivirta et al. 1999)
$log (P_L/Pa) = 12.89 – 6137/(T/K)$ (solid, Passivirta et al. 1999)
$log (P_L/Pa) = 9.08 – 3629/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
3.89 × 10⁻⁶, 3.55 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
$log (P_L/mmHg) = 32.22 – 6105/(T/K) – 7.332\log (T/K)$ (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
0.417 (calculated-SOFA model, Govers & Krop 1998)
$log [H/(Pa \cdot m³/mol)] = 7.40 – 1117/(T/K)$ (Passivirta et al. 1999)
1.26; 0.417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Chlorinated Dibenzofurans

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 7.43 (calculated-SOFA model, Govers & Krop 1998)
- 7.65 (estimated-solubility $S_L$ and regression eq. using lit. $K_{OW}$ values, Passivirta et al. 1999)
- 6.87; 7.43 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$ or log $K_B$:
- 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.91; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:
- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatileization:
- Photolysis: $t_\frac{1}{2} = 82.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH}(calc) = 0.74 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
  - $k_{OH} = (0.7 \text{–} 2.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
- $k_1 = 170$ L kg$^{-1}$ d$^{-1}$, 369 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for H$_6$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 > 2.0$ d$^{-1}$ (120-h exposure: metabolic inhibitor PBO-treated goldfish, Sijm et al. 1993)
- $k_1 = 1101$ L kg$^{-1}$ d$^{-1}$; $k_2 = 0.103$ d$^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
- $t_\frac{1}{2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_\frac{1}{2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: $t_\frac{1}{2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_\frac{1}{2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_\frac{1}{2} < 0.3$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).
9.1.1.28  2,3,4,6,7,8-Hexachlorodibenzofuran

Common Name: 2,3,4,6,7,8-Hexachlorodibenzofuran
Synonym: 2,3,4,6,7,8-HCDF
Chemical Name: 2,3,4,6,7,8-hexachlorodibenzofuran
CAS Registry No: 60851-34-5
Molecular Formula: C\textsubscript{12}H\textsubscript{2}Cl\textsubscript{6}O, C\textsubscript{6}HCl\textsubscript{3}OC\textsubscript{6}HCl\textsubscript{3}
Molecular Weight: 374.863
Melting Point (°C): 239–240 (Rordorf 1989)
Boiling Point (°C): 487.7 (calculated, Rordorf 1989)
Density (g/cm\textsuperscript{3}): 302.1 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm\textsuperscript{3}/mol):

- 302.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_\text{v}$ (kJ/mol):
- 85.7 (Rordorf 1989)

Enthalpy of Sublimation, $\Delta H_{\text{subl}}$ (kJ/mol):
- 136.794 (Rordorf 1989)

Enthalpy of Fusion, $\Delta H_\text{fus}$ (kJ/mol):
- 48.1 (Rordorf 1989)

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
- 94 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, $F$:
- 0.000276 (calculated, Passivirta et al. 1999)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations):
- 0.00156 (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
- $\log [S_L/(\text{mol/L})] = 0.787 - 2527/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $1.24 \times 10^{-1}, 1.56 \times 10^{-3}$ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- $5.82 \times 10^{-6}$ (supercooled liquid $P_L$, GC-RT correlation, Eitzer & Hites 1989)
- $3.88 \times 10^{-3}$ (corrected, supercooled liquid $P_L$, in Eitzer & Hites 1988, Eitzer & Hites 1998)
- $2.6 \times 10^{-5}, 1.9 \times 10^{-6}, 7.3 \times 10^{-5}, 1.7 \times 10^{-3}, 0.028$ (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
- $7.59 \times 10^{-6}$ (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
- $5.54 \times 10^{-5}, 1.53 \times 10^{-6}$ (supercooled liquid $P_L$ from GC-RT correlation; converted to solid $P_S$ with fugacity ratio $F$, Passivirta et al. 1999)
- $\log (P_L/Pa) = 12.91 - 6175/(T/K)$ (solid, Passivirta et al. 1999)
- $\log (P_L/Pa) = 8.00 - 3651/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\log (P_L/\text{mmHg}) = 31.99 - 6108/(T/K) - 7.332 \times \log (T/K)$ (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol or as indicated and reported temperature dependence equations):
- 1.78 (calculated-SOFA model, Govers & Krop 1998)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 7.21 - 1124/(T/K)$ (Passivirta et al. 1999)
- $1.26; 1.78$ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Chlorinated Dibenzofurans

Octanol/Water Partition Coefficient, log $K_{OW}$:
7.0 (calculated, Broman et al. 1991)
7.65 (calculated-SOFA model, Govers & Krop 1998)
7.62 (estimated-solubility $S_t$ and regression eq. using lit. $K_{OW}$ values, Passivirta et al. 1999)
6.937 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.01; 7.65 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated:
12.10 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log $K_B$:
4.88 (goldfish, 120-h exposure studies, Sijm et al. 1993)
4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid weight basis: measured-$C_{fish}/C_W$; calculated; rate constant ratio $k_1/k_2$ from non-linear regression analysis, Loonen et al. 1994b)
4.59 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.51 (fish muscle log BCF calculated from water, Wu et al. 2001)
4.81; 4.59 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:
6.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.96 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
9.10; 8.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:
Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_\frac{1}{2} = 2.8$ h for native congener (Tysklind & Rappe 1991);
$t_\frac{1}{2} = 70.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)
Oxidation: rate constant k, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH}$(calc) = 0.74 x 10$^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
$k_{OH} = (0.7 - 2.6) x 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of 1.5 x 10$^6$ molecule/cm$^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
$k_1 = 267$ L kg$^{-1}$ d$^{-1}$; $k_2 < 0.1$ d$^{-1}$ (goldfish after 120-h exposure: control fish, Sijm et al. 1993)
$k_2 = 0.36$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)
$k_1 = 110$ L kg$^{-1}$ d$^{-1}$, 174 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for P$_5$CDD homolog group, goldfish after 120-h exposure:
metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
$k_2 = 0.0119$ d$^{-1}$ with a biological $t_\frac{1}{2} = 25$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);
$t_\frac{1}{2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Surface water: $t_\frac{1}{2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Ground water:
Sediment: $t_\frac{1}{2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Soil: $t_\frac{1}{2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Biota: $t_\frac{1}{2} = 1.9$ d for PBO treated goldfish and $t_\frac{1}{2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993),
biological $t_\frac{1}{2} = 25$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
### 9.1.1.29 1,2,3,4,6,7,8-Heptachlorodibenzofuran

![Chemical Structure of 1,2,3,4,6,7,8-Heptachlorodibenzofuran](image)

**Common Name:** 1,2,3,4,6,7,8-Heptachlorodibenzofuran  
**Synonym:** 1,2,3,4,6,7,8-HCDF  
**Chemical Name:** 1,2,3,4,6,7,8-Heptachlorodibenzofuran  
**CAS Registry No:** 67562-39-4  
**Molecular Formula:** $\text{C}_{12}\text{HCl}_7\text{O}$, $\text{C}_6\text{HCl}_3\text{OC}_6\text{Cl}_4$  
**Molecular Weight:** 409.308

- **Melting Point (°C):** 236–237 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)
- **Boiling Point (°C):** 507.2 (calculated, Rordorf 1989)
- **Density (g/cm³ at 20°C):**  
  - 323.0 (calculated-Le Bas method at normal boiling point)
  - 238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
- **Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):**  
  - 87.8 (Rordorf 1989)
- **Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):**  
  - 144.642 (Rordorf 1989)
- **Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):**  
  - 53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
- **Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):**  
  - 106 (Rordorf 1989; quoted, Passivirta et al. 1999)
- **Fugacity Ratio at 25°C, F:**  
  - 0.000122 (calculated-$\Delta S_{fus}$ and mp, Passivirta et al. 1999)
- **Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):**  
  - $1.35 \times 10^{-6}$ (22.7°C, generator column-GC/MS, Friesen et al. 1990)
  - $1.08 \times 10^{-3}$ (calculated-QSAR, Fiedler & Schramm 1990)
  - $9.50 \times 10^{-7}$ (computed-expert system SPARC, Kollig 1995)
  - $1.26 \times 10^{-7}$ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  - $1.63 \times 10^{-4}$; $7.11 \times 10^{-4}$ (supercooled liquid $S_L$, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  - $\log [S_L/(\text{mol/L})] = 0.917 – 2812/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
  - $4.92 \times 10^{-4}$; $7.11 \times 10^{-4}$ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
- **Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
  - $1.93 \times 10^{-6}$ (supercooled liquid $P_L$, GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)
  - $4.7 \times 10^{-9}$; $4.3 \times 10^{-7}$; $2.0 \times 10^{-5}$; $5.8 \times 10^{-4}$; $1.1 \times 10^{-2}$ (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
  - $5.10 \times 10^{-8}$ (gas saturation method, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
  - $8.70 \times 10^{-9}$ (computed-expert system SPARC, Kollig 1995)
  - $1.83 \times 10^{-3}$; $1.58 \times 10^{-3}$ ($P_s$ solid vapor pressure calculated from reported $P_L$, Della Site 1997)
  - $1.84 \times 10^{-3}$ (corrected supercooled liquid $P_L$ in Eitzer & Hites 1988, Eitzer & Hites 1998)
  - $1.4 \times 10^{-6}$; $2.51 \times 10^{-6}$ (supercooled liquid $P_L$, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
  - $5.54 \times 10^{-5}$; $6.76 \times 10^{-5}$ (supercooled liquid $P_L$ from GC-RT correlation; converted to solid $P_s$ with fugacity ratio F, Passivirta et al. 1999)
log \( \frac{P}{Pa} \) = 12.98 – 6302/(T/K) (solid, Passivirta et al. 1999)
log \( \frac{P}{Pa} \) = 7.45 – 3486/(T/K) (supercooled liquid, Passivirta et al. 1999)
log \( \frac{P_{L}/mmHg}{Pa} \) = 30.03 – 6090/(T/K) – 6.798·log (T/K) (supercooled liquid \( P_{L} \), Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
9.33 × 10⁻³, 2.51 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry’s Law Constant (Pa m³/mol at 25°C):
3.80 (computed-expert system SPARC, Kollig 1995)
3.47; 1.41 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
log \[ \frac{H}{Pa m^3/mol} \] = 6.53 – 674/(T/K) (Passivirta et al. 1999)
1.41; 1.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
7.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989a)
9.25 (calculated-QSAR, Friedler & Schramm 1990)
7.90 (quoted, Loonen et al. 1991)
8.10 (calculated, Broman et al. 1991)
7.92 (recommended, Hansch et al. 1995)
8.52 (computed-expert system SPARC, Kollig 1995)
8.01 (calculated-SOFA model, Govers & Krop 1998)
8.07 (calculated-solubility log \( S_{L} \) and regression from lit. log \( K_{OW} \), Passivirta et al. 1999)
7.477 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
7.37; 8.00 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated:
12.06 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log \( BCF \):
4.46; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
4.46; 4.60; 4.63 (guppy, 21-d exposure, lipid wt basis: measured-\( C_{bio}/C_{w} \); calculated; rate constant ratio \( k_{1}/k_{2} \); from non-linear regression analysis, Loonen et al. 1994b)
4.46; 4.26 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
6.62; 6.92 (wet wt basis, fish 5% lipid, 10% lipid, Geyer et al. 2000)
5.89, 6.03 (fish muscle log BCFL calculated from water, sediment, Wu et al. 2001)
4.51; 4.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log \( K_{OC} \):
6.37 (organic carbon, calculated-QSAR, Friedler & Schramm 1990)
6.00 (organic carbon, calculated, Broman et al. 1991)
7.90 (calculated, Broman et al. 1991)
8.20 (computed-\( K_{OC} \), Kollig 1995)
9.64; 9.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):
Volatilization:
Photolytic degradation \( t_{1/2} = 9.8 \) h with extract of fly-ash and in tetradecane solution for native congener and \( t_{1/2} = 3.7 \) h for \(^{13}\text{C}\)-labelled congener (Tysklind & Rappe 1991).
\( t_{1/2} = 84.5 \) h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures see reference:
k_{O_3(aq.)} = 1.08 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}, \text{ oxidative degradation rate constant of water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987) k_{OH(calc)} = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1991) k_{OH}} = (0.5 – 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime } \tau = 17–31 \text{ d, using a 12-h average daytime OH radical concn of } 1.5 \times 10^6 \text{ molecule/cm}^3 \text{ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991) }

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 42, 61 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.43, 0.1 \text{ d}^{-1} \text{ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993) k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}, 61 \text{ L kg}^{-1} \text{ d}^{-1} \text{ (average } k_1 \text{ for P}_5\text{CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993) k_2 = 0.0084 \text{ d}^{-1} \text{ with a biological } t_{02} = 36 \text{ d (blue mussel, 99-d exposure, Hektoen et al. 1994) k_1 = 524 \text{ L kg}^{-1} \text{ d}^{-1}; k_2 = 0.127 \text{ d}^{-1} \text{ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b) }

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radicals to be 17–31 d (Atkinson 1991); 

\[ t_{1/2} = 3200 \text{ h at } 7^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \]

Surface water: \[ t_{1/2} = 64000 \text{ h at } 7^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \]

Groundwater:

Sediment: very persistent \[ t_{1/2} > 36 \text{ yr (Geyer et al. 2000) } \]

degradation \[ t_{1/2} = 2–200 \text{ yr for all homologues (estimated, Suzuki et al. 2000);} \]

\[ t_{1/2} = 350000 \text{ h at } 7^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \]

Soil: degradation \[ t_{1/2} = 5–50 \text{ yr (estimated, Suzuki et al. 2000);} \]

\[ t_{1/2} = 350000 \text{ h at } 7^\circ \text{C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).} \]

Biota: depuration \[ t_{1/2} > 336 \text{ d for carp in Lake Superior water (Kuehl et al. 1987);} \]

elimination \[ t_{1/2} = 33.9 \text{ d from lactating cow (Olling et al. 1991);} \]

\[ t_{1/2} = 1.6 \text{ d for PBO treated goldfish and } t_{1/2} = 6.8 \text{ d for control fish in 120-h exposure studies (Sijm et al. 1993).} \]

\[ t_{1/2} = 37 \text{ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994) } \]
**9.1.1.30  1,2,3,4,6,8,9-Heptachlorodibenzofuran**

![Chemical structure of 1,2,3,4,6,8,9-Heptachlorodibenzofuran](image)

Common Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran
Synonym: 1,2,3,4,6,8,9-HpCDF
Chemical Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran
CAS Registry No: 69698-58-4
Molecular Formula: C_{12}HCl_{7}O, C_{6}HCl_{3}OC_{6}Cl_{4}
Molecular Weight: 409.308
Melting Point (°C):
211–212 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):
323.0 (calculated-Le Bas method)
238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
89.2 (Rordorf 1989)
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
145.64 (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
111 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, $F$:
0.00021 (calculated-$\Delta S_{fus}$ and mp, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
5.65 $\times$ 10^{-4} (supercooled liquid $S_L$, calculated-SOFA model, Govers & Krop 1998)
log $[S_L$/mol/L] = 1.200 – 2861/(T/K), (supercooled liquid, Passivirta et al. 1999)
4.19 $\times$ 10^{-4}, 5.65 $\times$ 10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7.7 $\times$ 10^{-9}, 7.2 $\times$ 10^{-7}, 3.6 $\times$ 10^{-5}, 1.0 $\times$ 10^{-3}, 2.0 $\times$ 10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1989)
7.24 $\times$ 10^{-7} (supercooled liquid $P_L$, calculated-SOFA model, Govers & Krop 1998)
1.55 $\times$ 10^{-3}, 3.57 $\times$ 10^{-9} (supercooled liquid $P_L$ from GC-RT correlation; converted to solid $P_S$ with fugacity ratio $F$, Passivirta et al. 1999)
log ($P_L$/Pa) = 13.03 – 6394/(T/K), (solid, Passivirta et al. 1999)
log ($P_L$/Pa) = 7.23 – 3581/(T/K), (supercooled liquid, Passivirta et al. 1999)
log ($P_L$/mmHg) = 29.94 – 6089/(T/K) – 6.798·log (T/K) (supercooled liquid $P_L$, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
5.13 (calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m³/mol)] = 6.03 – 756/(T/K), (Passivirta et al. 1999)
1.45; 5.13 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 8.02 (calculated-SOFA model, Govers & Krop 1998)
- 7.91 (calculated-solubility log $S_L$ and regression from lit. log $K_{OW}$, Passivirta et al. 1999)
- 7.43; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- 4.42 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.46; 4.42 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatileization:
Photolysis: $t_{1/2} = 85.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{OH}\text{(calc)} = 0.53 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (0.5 - 0.9) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6$ molecule/cm$^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 42$ L kg$^{-1}$ d$^{-1}$, 61 L kg$^{-1}$ d$^{-1}$ (average $k_1$ for H$_7$CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radical to be 17–31 d (Atkinson 1991);
- suggested $t_{1/2} = 3200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: suggested $t_{1/2} = 64000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: degradation $t_{1/2} = 2$–200 yr for all homologues (estimated, Suzuki et al. 2000);
- suggested $t_{1/2} = 350000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).
Soil: degradation $t_{1/2} = 5$–50 yr (estimated, Suzuki et al. 2000);
- suggested $t_{1/2} = 350000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota:
9.1.1.31 1,2,3,4,7,8,9-Heptachlorodibenzofuran

Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
Synonym: 1,2,3,4,7,8,9-HCDF
Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
CAS Registry No: 55673-89-7
Molecular Formula: C₁₂HCl₇O, C₆HCl₃OC₆Cl₄
Molecular Weight: 409.308
Melting Point (°C):
221–223 (Kuroki et al. 1984)
Boiling Point (°C):
507.2 (calculated, Rordorf 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
323.0 (calculated-Le Bas method at normal boiling point)
248.1 (Passivirta et al. 1999)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
88.6 (Rordorf 1989)
Enthalpy of Sublimation, ∆Hₘₛₘ (kJ/mol):
145.221 (Rordorf 1989)
Enthalpy of Fusion, ∆Hₖ₃ (kJ/mol):
53.9 (Rordorf 1989)
Entropy of Fusion, ∆Sₖ₃ (J/mol K):
109 (Rordorf 1989; quoted, Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.000179 (calculated-∆Sₖ₃ and mp, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
1.30 × 10⁻⁶ (computed-expert system SPARC, Kollig 1995)
2.58 × 10⁻⁴ (supercooled liquid Sₗ, calculated-SOFA model, Govers & Krop 1998)
log [Sₗ/(mol/L)] = 1.100 – 2819/(T/K) (supercooled liquid, Passivirta et al. 1999)
2.83 × 10⁻⁴, 2.58 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.2 × 10⁻⁶, 5.8 × 10⁻⁷, 2.8 × 10⁻⁵, 8.0 × 10⁻⁴, 1.5 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
1.305 × 10⁻⁴ (supercooled liquid Pₛ, GC-RT correlation, Eitzer & Hites 1988, 1991)
1.011 × 10⁻⁴ (supercooled liquid Pₛ, GC-RT correlation, Eitzer & Hites 1989)
1.27 × 10⁻⁹ (computed-expert system SPARC, Kollig 1995)
1.48 × 10⁻⁴, 1.14 × 10⁻³ (solid vapor pressures calculated from reported Pₛ, Della Site 1997)
6.61 × 10⁻⁷ (supercooled liquid Pₛ, calculated-SOFA model, Govers & Krop 1998)
7.87 × 10⁻⁶; 1.41 × 10⁻⁶ (supercooled liquid Pₛ from GC-RT correlation; converted to solid Pₛ with fugacity ratio F, Passivirta et al. 1999)
log (Pₛ/Pa) = 13.12 – 6547/(T/K) (solid, Passivirta et al. 1999)
log (Pₛ/Pa) = 7.23 – 3581/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (Pₛ/mmHg) = 29.69 – 6089/(T/K) – 6.798·log (T/K) (supercooled liquid Pₛ, Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
5.75 × 10⁻², 6.60 × 10⁻² (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)
Henry’s Law Constant (Pa m³/mol or as indicated and reported temperature dependence equations):

- 3.85 (computed-expert system SPARC, Kollig 1995)
- 1.0 (calculated-SOFA model, Govers & Krop 1998)

\[ \log \left[ \frac{H}{(Pa \ m^3/mol)} \right] = 6.32 - \frac{912}{(T/K)} \] (Passivirta et al. 1999)

- 1.58; 1.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log \( K_{ow} \):

- 6.90 (calculated, Broman et al. 1991)
- 8.50 (computed-expert system SPARC, Kollig 1995)
- 8.23 (calculated-SOFA model, Govers & Krop 1998)
- 7.99 (calculated-solubility log \( S_L \) and regression from lit. log \( K_{ow} \), Passivirta et al. 1999)
- 7.616 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.60; 8.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25 °C or as indicated:

- 12.34 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log \( BCF \):

- 4.32 (calculated-SOFA model, Govers & Krop 1998)
- 5.59 (fish muscle log \( BCF_L \) calculated from water, Wu et al. 2001)
- 4.30; 4.32 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log \( K_{oc} \):

- 5.00 (organic carbon, calculated, Broman et al. 1991)
- 6.70 (calculated, Broman et al. 1991)
- 8.23 (computed- \( K_{ow} \), Kollig 1995)

Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis: photolysis \( t_{1/2} = 3.3 \) h in the extract from fly ash in tetradecane, for 13C labelled congener (Tysklind & Rappe 1991)

\( t_{1/2} = 84.5 \) h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{oh} \) for reaction with OH radical, \( k_{no3} \) with NO_3 radical and \( k_{o3} \) with O_3 as indicated, *data at other temperatures see reference:

\( k_{oh} \) (calc) = 0.92 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

\( k_{oh} = (0.5 - 0.9) \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of 1.5 × 10^6 molecule/cm³ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\( k_1 = 42 \) L kg⁻¹ d⁻¹, 61 L kg⁻¹ d⁻¹ (average \( k_1 \) for H,CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF, with OH radicals to be 17–31 d (Atkinson 1991);

\( t_{1/2} = 3200 \) h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: \( t_{1/2} = 64 \) 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Chlorinated Dibenzofurans

Groundwater:
Sediment: degradation $t_{1/2} = 20–200$ y for all homologues (estimated, Suzuki et al. 2000);
$t_{1/2} = 300,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: degradation $t_{1/2} = 5–50$ yr (estimated, Suzuki et al. 2000);
$t_{1/2} = 300,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota:
### Octachlorodibenzofuran

**Common Name:** Octachlorodibenzofuran  
**Synonym:** OCDF  
**Chemical Name:** octachlorodibenzofuran  
**CAS Registry No:** 39001-02-0  
**Molecular Formula:** C₁₂Cl₄OC₆Cl₄  
**Molecular Weight:** 443.753

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>258–260</td>
<td>Rordorf 1986,1989</td>
</tr>
<tr>
<td></td>
<td>259</td>
<td>Ruelle &amp; Kesselring 1997, Passivirta et al. 1999</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>510</td>
<td>(calculated, Rordorf 1986)</td>
</tr>
<tr>
<td></td>
<td>537</td>
<td>(calculated, Rordorf 1989)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>343.9</td>
<td>(calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td></td>
<td>251.0</td>
<td>(Ruelle &amp; Kesselring 1997, quoted, Passivirta et al. 1999)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, ΔHᵥ (kJ/mol)</td>
<td>90</td>
<td>Rordorf 1989</td>
</tr>
<tr>
<td>Enthalpy of Sublimation, ΔHₛₐₙ l (kJ/mol)</td>
<td>149.43</td>
<td>Rordorf 1989</td>
</tr>
<tr>
<td></td>
<td>284.38</td>
<td>(Dickhut et al. 1994)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔHₛₐₙ (kJ/mol)</td>
<td>57.5</td>
<td>Rordorf 1989; quoted, Ruelle &amp; Kesselring 1997</td>
</tr>
<tr>
<td>Entropy of Fusion, ΔSₛₐₙ (J/mol K)</td>
<td>108</td>
<td>Rordorf 1986,1989; quoted, Passivirta et al. 1999</td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C, F</td>
<td>0.00518</td>
<td>(calculated-assuming ΔSₛₐₙ = 56 J/mol K and mp = 258°C)</td>
</tr>
<tr>
<td></td>
<td>0.000037</td>
<td>(calculated- ΔSₛₐₙ and mp, Passivirta et al. 1999)</td>
</tr>
</tbody>
</table>

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (S)</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>39.8–80</td>
<td>1.16 × 10⁻⁶</td>
<td>log [S] = 0.081·t/°C (generator column-GC/ECD, temp range 40–80°C, Doucette &amp; Andren 1988a)</td>
</tr>
<tr>
<td>40–80</td>
<td>1.37 × 10⁻⁶</td>
<td>[S] = 0.5720 – 3008/(T/K) (supercooled liquid, Passivirta et al. 1999)</td>
</tr>
</tbody>
</table>

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (P)</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>39.8–80</td>
<td>5.00 × 10⁻¹⁰</td>
<td>log [P] = -5.0496 – 7455.1/(T/K) (regression eq. of literature data, Shiu &amp; Ma 2000)</td>
</tr>
<tr>
<td>30–50</td>
<td>3.43 × 10⁻⁷</td>
<td>[P] = 0.5720 – 3008/(T/K) (supercooled liquid, Passivirta et al. 1999)</td>
</tr>
</tbody>
</table>
Chlorinated Dibenzo-2243

0.000221* (105.6 °C, average value, gas saturation-GC, measured range 105.6–261.2 °C, Rordorf 1990)
5.00 × 10⁻¹⁰ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
1.26 × 10⁻⁹ (solid vapor pressure calculated from reported P_L, Delle Site 1997)
7.08 × 10⁻⁶; 1.82 × 10⁻⁶ (supercooled liquid P_L, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
1.30 × 10⁻⁶; 4.83 × 10⁻¹¹ (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

log (P_Pa) = 13.42 – 7073/(T/K) (solid, Passivirta et al. 1999)
log (P_Pa) = 7.77 – 4068/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry’s Law Constant (Pa m³/mol or as indicated and reported temperature dependence equations):
0.10 (estimated, Clark & Mackay 1991)
1.31; 0.776 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
log [H/(Pa m³/mol)] = 7.20 – 1060/(T/K) (Passivirta et al. 1999)
2.14; 0.776 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_OW:
13.06, 13.22, 13.78; 12.54, 13.37, 13.93 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
8.78 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
7.97 (generator column-GC/ECD, Doucette & Andren 1987, 1988b)
7.90 (HPLC-RT correlation, Doucette & Andren 1988b)
7.97 (recommended, Hansch et al. 1995)
8.78; 8.60 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
8.62 (calculated-solubility log S_i and regression from lit. log K_OW, Passivirta et al. 1999)
7.992 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
8.03; 8.60 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_OA at 25°C or as indicated:
12.84 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF:
1.613, 0.70 (human fat, calculated-different K_OWS, wet weight basis, Geyer et al. 1987)
1.71, 0.778 (human fat, calculated-different K_OWS, lipid basis, Geyer et al. 1987)
2.77; 3.89 (guppy, wet weight based; lipid weight based, Gobas & Schrap 1990)
3.90; 4.10; 4.11 (guppies, 21-d exposure, lipid wt basis: measured-C_fish/C_W; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
3.90; 3.88 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
7.48; 7.78 (wet wt basis: fish with 5% lipid, with 10% lipid, Geyer et al. 2000)
7.61, 7.63 (fish muscle log BCF_L calculated from water, sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_OC:
6.75 (calculated-QSAR, Fiedler & Schramm 1990)
6.00 (organic carbon, calculated, Broman et al. 1991)
7.40 (calculated, Broman et al. 1991)
7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
8.13, 8.48 (calculated-K_OC, Kollig 1993)
10.49; 10.30 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization:
Photolysis: photolytic t½ = 2.1 h from extract of fly ash in tetrade cane solution for native congener (Tysklind & Rappe 1991);
photolysis k = 2.7 × 10⁻³ min⁻¹ with t½ = 260 min in pure water and t½ = 6.3 × 10⁻³ min⁻¹ with t½ = 110 min in 60% acetonitrile/water at 300 nm photochemical reactor; k = 0.11 h⁻¹ with t½ = 6.5 h in pure water in sunlight at 42°N latitude in middle of July (Kim & O’Keefe 2000).
t½ = 100.5 h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO₃ with NO₃ radical and kO₃ with O₃ or as indicated, *data at other temperatures see reference:
k (oxidative degradation rate constant of water dissolved OCDF by ozone) is 1.05 × 10⁴ L g⁻¹ min⁻¹ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)
kOH(calc) = 0.39 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)
kOH = 0.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with calculated tropospheric lifetime τ = 39 d, using a 12-h average daytime OH radical concn of 1.5 × 10⁶ molecule/cm³ for OCDF at room temp. (Atkinson 1991)
photodegradation t½ = 9 h for OCDF adsorbed to clean silica gels in a rotary photo-reactor by filtered < 290 nm of light (Koester & Hites 1992)

Biodegradation:
Bioremediation: metabolism half-time 10⁷ h (guppy, Clark & Mackay 1991).

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
k₂ = 0.012 d⁻¹ (rainbow trout, Niimi & Oliver 1986)
k₁ = 824 d⁻¹; k₂ = 1.40 d⁻¹ (guppy, Gobas & Schrap 1990)
k₁ = 0.0101 d⁻¹ with a biological t½ = 30 d (blue mussel, 99-d exposure, Hektoen et al. 1994)
k = 217 L kg⁻¹ d⁻¹; k₂ = 0.174 d⁻¹ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:
Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for OCDF with OH radicals to be 39 d (Atkinson 1991);
t½ = 9600 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: photolysis k = 2.7 × 10⁻³ min⁻¹ with t½ = 260 min in pure water and k = 6.3 × 10⁻³ min⁻¹ with t½ = 110 min in 60% acetonitrile/water at 300 nm photochemical reactor; k = 0.11 h⁻¹ with a t½ = 6.5 h in pure water in sunlight at 42°N latitude in middle of July (Kim & O’Keefe 2000);
t½ = 192000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: very persistent t½ = 29 yr (Geyer et al. 2000)
degradation t½ = 20–200 yr for all homologues (estimated, Suzuki et al. 2000);
t½ = 250 000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: degradation t½ = 5–50 yr (estimated, Suzuki et al. 2000);
t½ = 250000 h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: mean biological t½ = 7 d in rainbow trout (Niimi 1986)
t½ = 7 to 12 d in rainbow trout (Niimi & Oliver 1986)
biological t½ = 30 d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)
TABLE 9.1.32.1
Reported aqueous solubilities and vapor pressures of octachlorodibenzofuran at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Doucette &amp; Andren 1988a</strong></td>
<td><strong>Rordorf 1987, 1989</strong></td>
</tr>
<tr>
<td>generator column-GC/ECD</td>
<td>gas saturation-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>39.5</td>
<td>3.85×10⁻⁶</td>
</tr>
<tr>
<td>56.6</td>
<td>1.40×10⁻⁵</td>
</tr>
<tr>
<td>80.0</td>
<td>5.86×10⁻⁵</td>
</tr>
<tr>
<td>25.0</td>
<td>1.16×10⁻⁶</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>S/(mol/L) = a·exp[b·(t/°C)]</td>
<td>ΔH_u/(kJ mol⁻¹) = 90.0</td>
</tr>
<tr>
<td>a</td>
<td>5.87×10⁻¹³</td>
</tr>
<tr>
<td>b</td>
<td>0.068</td>
</tr>
<tr>
<td>ΔH_fus/(kJ mol⁻¹) = 53.35</td>
<td>ΔS_fus/(J mol⁻¹ K⁻¹) = 90.0</td>
</tr>
<tr>
<td>5–45°C</td>
<td></td>
</tr>
</tbody>
</table>

© 2006 by Taylor & Francis Group, LLC

ΔH_sub/(kJ mol⁻¹) = 143.702
105–261°C
FIGURE 9.1.32.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for octachlorodibenzofuran.
### 9.2 SUMMARY TABLES AND QSPR PLOTS

**TABLE 9.2.1**
Summary of physical properties of some chlorinated furans

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Chlorine no. n</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Le Bas molar volume $V_m$ cm$^3$/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibenzofuran</td>
<td>132-64-9</td>
<td>$C_{12}H_8O$</td>
<td>0</td>
<td>168.191</td>
<td>86.5</td>
<td>287</td>
<td>0.249</td>
<td>176.1</td>
</tr>
<tr>
<td>2-Chloro-</td>
<td>51230–49–0</td>
<td>$C_{12}H_7OCl$</td>
<td>1</td>
<td>202.637</td>
<td>101.5–102.5</td>
<td>338.2</td>
<td>0.175</td>
<td>197.6</td>
</tr>
<tr>
<td>3-Chloro-</td>
<td>25074–67–3</td>
<td>$C_{12}H_7OCl$</td>
<td>1</td>
<td>202.637</td>
<td>101–102</td>
<td>338.2</td>
<td>0.178</td>
<td>197.6</td>
</tr>
<tr>
<td>2,3-Dichloro-</td>
<td>64126–86–9</td>
<td>$C_{12}H_6OCl_2$</td>
<td>2</td>
<td>237.082</td>
<td>125.5–127</td>
<td>375.0</td>
<td>0.102</td>
<td>218.5</td>
</tr>
<tr>
<td>2,7-Dichloro-</td>
<td>73992–98–6</td>
<td>$C_{12}H_6OCl_2$</td>
<td>2</td>
<td>237.082</td>
<td>184–185</td>
<td>375</td>
<td>0.0272</td>
<td>218.5</td>
</tr>
<tr>
<td>2,8-Dichloro-</td>
<td>5409–83–6</td>
<td>$C_{12}H_6OCl_2$</td>
<td>2</td>
<td>237.082</td>
<td>188</td>
<td>375</td>
<td>0.0252</td>
<td>218.5</td>
</tr>
<tr>
<td>3,6-Dichloro-</td>
<td>94570–83–9</td>
<td>$C_{12}H_6OCl_2$</td>
<td>2</td>
<td>237.082</td>
<td>189–191</td>
<td>408.4</td>
<td>0.0240</td>
<td>239.4</td>
</tr>
<tr>
<td>2,3,3-Trichloro-</td>
<td>57117–32–5</td>
<td>$C_{12}H_5OCl_3$</td>
<td>3</td>
<td>271.527</td>
<td>116–117</td>
<td>408.4</td>
<td>0.126</td>
<td>239.4</td>
</tr>
<tr>
<td>2,4,6-Trichloro-</td>
<td>58802–14–5</td>
<td>$C_{12}H_5OCl_3$</td>
<td>3</td>
<td>271.527</td>
<td>154</td>
<td>392.5</td>
<td>0.0542</td>
<td>239.4</td>
</tr>
<tr>
<td>2,4,8-Trichloro-</td>
<td>54589–71–8</td>
<td>$C_{12}H_5OCl_3$</td>
<td>3</td>
<td>271.527</td>
<td>210–211</td>
<td>438.3</td>
<td>0.0151</td>
<td>260.3</td>
</tr>
<tr>
<td>1,2,3,4-Tetrachloro-</td>
<td>24478–72–6</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>168.5–169</td>
<td>438.3</td>
<td>0.0389</td>
<td>260.3</td>
</tr>
<tr>
<td>1,2,3,7-Tetrachloro-</td>
<td>83704–22–7</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>167.5–168</td>
<td>438.3</td>
<td>0.0398</td>
<td>260.3</td>
</tr>
<tr>
<td>1,2,7,8-Tetrachloro-</td>
<td>58802–20–3</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>177–178</td>
<td>438.3</td>
<td>0.0319</td>
<td>260.3</td>
</tr>
<tr>
<td>1,3,6,8-Tetrachloro-</td>
<td>71998–72–6</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>206.5–207.5</td>
<td>438.3</td>
<td>0.0168</td>
<td>260.3</td>
</tr>
<tr>
<td>1,3,7,8-Tetrachloro-</td>
<td>57117–35–8</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>227</td>
<td>438.3</td>
<td>0.0104</td>
<td>260.3</td>
</tr>
<tr>
<td>1,3,7,9-Tetrachloro-</td>
<td>64650–17–4</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>225–227</td>
<td>464.7</td>
<td>0.0107</td>
<td>281.2</td>
</tr>
<tr>
<td>2,3,7,8-Tetrachloro-</td>
<td>51207–31–9</td>
<td>$C_{12}H_4OCl_4$</td>
<td>4</td>
<td>305.978</td>
<td>226</td>
<td>487.7</td>
<td>0.017</td>
<td>281.2</td>
</tr>
<tr>
<td>1,2,3,4,7-Pentachloro-</td>
<td>83704–48–7</td>
<td>$C_{12}H_3OCl_5$</td>
<td>5</td>
<td>340.418</td>
<td>223–234</td>
<td>487.7</td>
<td>0.00895</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,7,8-Pentachloro-</td>
<td>57117–41–6</td>
<td>$C_{12}H_3OCl_5$</td>
<td>5</td>
<td>340.418</td>
<td>226</td>
<td>487.7</td>
<td>0.0132</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,4,7,8-Pentachloro-</td>
<td>83704–51–2</td>
<td>$C_{12}H_3OCl_5$</td>
<td>5</td>
<td>340.418</td>
<td>196–196.5</td>
<td>464.7</td>
<td>0.00832</td>
<td>302.1</td>
</tr>
<tr>
<td>2,3,4,7,8-Pentachloro-</td>
<td>57117–31–4</td>
<td>$C_{12}H_3OCl_5$</td>
<td>5</td>
<td>340.418</td>
<td>216–217</td>
<td>487.7</td>
<td>0.00656</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,4,6,8-Hexachloro-</td>
<td>69698–60–8</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>233–234</td>
<td>487.7</td>
<td>0.00656</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,4,7,8-Hexachloro-</td>
<td>70658–26–9</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>222</td>
<td>487.7</td>
<td>0.0118</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,4,7,9-Hexachloro-</td>
<td>91538–84–0</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>226</td>
<td>487.7</td>
<td>0.00910</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,6,7,8-Hexachloro-</td>
<td>57117–44–9</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>216–234</td>
<td>487.7</td>
<td>0.00566</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,7,8,9-Hexachloro-</td>
<td>72918–21–9</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>221–222</td>
<td>487.7</td>
<td>0.0118</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,4,6,7,8-Hexachloro-</td>
<td>67562–40–7</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>246–248</td>
<td>487.7</td>
<td>0.00664</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,4,6,8,9-Hexachloro-</td>
<td>68698–59–5</td>
<td>$C_{12}H_2OCl_6$</td>
<td>6</td>
<td>374.863</td>
<td>246–248</td>
<td>487.7</td>
<td>0.00664</td>
<td>302.1</td>
</tr>
</tbody>
</table>

*Continued*
<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Chlorine no. n</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Le Bas molar volume V_m cm³/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3,4,6,7,8-Hexachloro-</td>
<td>60851–34–5</td>
<td>C₁₂H₂OCl₆</td>
<td>6</td>
<td>374.863</td>
<td>239–240</td>
<td>487.7</td>
<td>0.00786</td>
<td>302.1</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-Heptachloro-</td>
<td>67462–39–4</td>
<td>C₁₂HOCl₇</td>
<td>7</td>
<td>409.308</td>
<td>236–237</td>
<td>507.2</td>
<td>0.00841</td>
<td>323.0</td>
</tr>
<tr>
<td>1,2,3,4,6,8,9-Heptachloro-</td>
<td>69698–58–4</td>
<td>C₁₂HOCl₇</td>
<td>7</td>
<td>409.308</td>
<td>211–212</td>
<td>507.2</td>
<td>0.0148</td>
<td>323.0</td>
</tr>
<tr>
<td>1,2,3,4,7,8,9-Heptachloro-</td>
<td>55673–89–7</td>
<td>C₁₂HOCl₇</td>
<td>7</td>
<td>409.308</td>
<td>221–223</td>
<td>507.2</td>
<td>0.0117</td>
<td>323.0</td>
</tr>
<tr>
<td>Octachlorodibenzofuran</td>
<td>39001–02–0</td>
<td>C₁₀OCl₈</td>
<td>8</td>
<td>443.753</td>
<td>258</td>
<td>537</td>
<td>0.00518</td>
<td>343.9</td>
</tr>
</tbody>
</table>

* Assuming ΔS_m = 56 J/mol K.
### TABLE 9.2.2
Selected physical-chemical properties of some chlorinated furans at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry’s law const.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P&lt;sub&gt;v&lt;/sub&gt;/Pa</td>
<td>P&lt;sub&gt;L&lt;/sub&gt;/Pa</td>
<td>S/(mg/m&lt;sup&gt;3&lt;/sup&gt;)</td>
</tr>
<tr>
<td>Dibenzofuran</td>
<td>0.400</td>
<td>1.606</td>
<td>4750</td>
</tr>
<tr>
<td>2,8-DCDF</td>
<td>0.00039</td>
<td>1.46×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>14.5</td>
</tr>
<tr>
<td>3,6-DCDF</td>
<td>2.00×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>7.94×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>7.95×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,3,8-T&lt;sub&gt;3&lt;/sub&gt;CDF</td>
<td>2.48×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>7.29×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>7.29×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,4,6-T&lt;sub&gt;3&lt;/sub&gt;CDF</td>
<td>9.22×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>7.29×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>7.29×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,4,8-T&lt;sub&gt;3&lt;/sub&gt;CDF</td>
<td>9.1×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>1.68×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>1.68×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>1,3,7,8-T&lt;sub&gt;4&lt;/sub&gt;CDF</td>
<td>3.51×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>6.39</td>
<td>6.39</td>
</tr>
<tr>
<td>2,3,7,8-T&lt;sub&gt;4&lt;/sub&gt;CDF</td>
<td>2.00×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>1.29×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>1.29×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>2,3,4,7,8-P&lt;sub&gt;5&lt;/sub&gt;CDF</td>
<td>3.50×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>1.68×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>1.68×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>1,2,3,4,7,8-H&lt;sub&gt;5&lt;/sub&gt;CDF</td>
<td>3.20×10&lt;sup&gt;-8&lt;/sup&gt;</td>
<td>2.30×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>2.30×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-H&lt;sub&gt;7&lt;/sub&gt;CDF</td>
<td>4.70×10&lt;sup&gt;-9&lt;/sup&gt;</td>
<td>3.59×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>3.59×10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>OCDF</td>
<td>5.0×10&lt;sup&gt;-10&lt;/sup&gt;</td>
<td>9.65×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>9.65×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

### TABLE 9.2.3
Suggested half-life classes of polychlorinated dibenzofurans in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibenzofuran</td>
<td>3</td>
<td>4</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>2,8-Dichloro-</td>
<td>4</td>
<td>5</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>2,3,7,8-TetraCloro-</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>2,3,4,7,8-PentaCloro-</td>
<td>5</td>
<td>5</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-HeptaCloro-</td>
<td>5</td>
<td>6</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>Octachlorodibenzofuran</td>
<td>5</td>
<td>7</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

where,

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>&lt;10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~ 1 day)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~ 2 days)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5500 (~ 8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17000 (~ 2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55000 (~ 6 years)</td>
<td>&gt;30,000</td>
</tr>
</tbody>
</table>
FIGURE 9.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

FIGURE 9.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.
FIGURE 9.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzofurans.

FIGURE 9.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzofurans.
FIGURE 9.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzofurans.
9.3 REFERENCES

References


Fletcher, C.L., McKay, W.A. (1993) Polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) in the aquatic environment - A literature review. *Chemosphere* 26, 1041–1069.


Sangster, J. (1993) LOGKOW Databank, Sangster Research Laboratories, Montreal, Quebec, Canada.


