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

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Kuo-Ching Ma
Sum Chi Lee

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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.

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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.
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16.1 LIST OF CHEMICALS AND DATA COMPILATIONS

16.1.1 NITRILES (ORGANIC CYANIDES)

16.1.1.1 Acetonitrile

Common Name: Acetonitrile
Synonym: cyanomethane, ethanenitrile, methyl cyanide
Chemical Name: acetonitrile
CAS Registry No: 75-05-8
Molecular Formula: C2H3N, CH3CN
Molecular Weight: 41.052
Melting Point (°C):
-43.82 (Lide 2003)
Boiling Point (°C):
81.65 (Lide 2003)
Density (g/cm³ at 20°C):
0.7857 (Dreisbach 1961; Weast 1982–83; Dean 1985)
0.7803 (25°C, Dreisbach 1961)
Molar Volume (cm³/mol):
52.7 (calculated-density, Rohrschneider 1973)
57.4 (exptl. at normal bp, Lee et al. 1972)
56.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
29.1 (pKₐ, Riddick et al. 1986; Howard 1993)
32.2 (pKₐ, Riddick et al. 1986)
-10.12 (pKₐH+, Riddick et al. 1986)
Enthalpy of Vaporization, ∆HV (kJ/mol):
35.01, 31.51 (25°C, bp, Dreisbach 1961)
32.94, 29.82 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
8.167 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
> 3.1 × 10⁶ (Booth & Everson 1948)
miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990; Howard 1993)
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):
11870* (interpolated-regression of tabulated data, temp range −47–81.8°C, Stull 1947)
log (P/mmHg) = 7.12257 − 1315.2/(230 + t/°C), (Antoine eq., Dreisbach & Martin 1949)
11240 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.07354 − 1279.2/(224.0 + t/°C), temp range 5–119°C, (Antoine eq. for liquid state, Dreisbach 1961)
12156* (25.56°C, measured range 7.3–27.38°C, Putnam et al. 1965)
log (P/mmHg) = 7.89511 − 1773.06/(T/K); temp range 280–300.5 K (Antoine eq., Putnam et al. 1965)
11510 (Hoy 1970)
24459* (41.82°C, ebulliometry, measured range 41–82°C, Meyer et al. 1971)
log (P/mmHg) = 6.23655 − 1397.9228/(239.275 + t/°C); temp range 41–82°C (ebulliometry, Meyer et al. 1971)
log (P/mmHg) = [−0.2185 × 8173.2/(T/K)] + 7.938662; temp range: −47.0 to 81.8°C, (Antoine eq., Weast 1972–73)
11919* (25.3°C, measured range 15.1–89.2°C, Dojcanske & Heinrich 1974)
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):

3.50, 2.78 (exptl., calculated-bond contribution, Hine & Mookerjee 1975)
2.07* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
2.033 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1.474* (20°C, headspace-GC, measured range 6.0–30°C, Benkelberg et al. 1995)
1.474, 1.477, 1.685 (20°C, headspace-GC, deionized water, rain water, artificial seawater, Benkelberg et al. 1995)

ln (K₀/atm) = (13.8 ± 0.3) – (4106 ± 101)/T/K, temp range: 6–30°C (headspace-GC measurement, Benkelberg et al. 1995)

1.55 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log Kᵦᵢ = 2.353 – 1627/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
2.05 (Ostwald concentration coefficient-concn ratio-GC/FID, Bebahani et al. 2002)

Octanol/Water Partition Coefficient, log Kₐₖᵢ:

–0.34 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969, 1971; Hansch & Leo 1985)
–0.54 (shake flask-GC, Tanii & Hashimoto 1984)
–0.34 (recommended, Sangster 1989, 1993)
–0.34 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₐₐᵢ:

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

Bioconcentration Factor, log BCF:

–0.523 (estimated-Kₐₖᵢ as per regression eq of Bysshe 1982, Howard 1993)

Sorption Partition Coefficient, log Kₒᵦ:

–0.523 (soil, estimated-Kₐₖᵢ, Lyman et al. 1982; quoted, Howard 1993)
–0.714 (calculated-Kₐₖᵢ, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, tᵢᵢ:

Volatilization: tᵢᵢ ~ 21 h from a model river of 1-m deep flowing at 1 m/s with a wind velocity of 3 m/s based
on Henry’s law constant (Lyman et al. 1982; quoted, Howard 1993)
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 and/or the Arrhenius expression see reference:
photooxidation $t_{1/2} = 314 – 12559$ yr in water, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)
$k_{OH} = (4.94 ± 0.6) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297.2 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Harris et al. 1981; quoted, Howard 1993)
$k_{OH}^* = (1.94 ± 0.37) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 250–363 K (flash photolysis-resonance fluorescence, Kurylo & Knable 1984)
$k_{OH}(exptl) = 2.1 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K, measured range 295–393 K (discharge flow-EPR, Poulet et al. 1984)
$k_{OH}(calc) = 2.0 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1985)
$k_{OH} = 3 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993)
$k_{OH}^* = 2.14 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

$k = 5.8 \times 10^{-3}$ M$^{-1}$ h$^{-1}$ at pH 7 and 25°C with $t_{1/2} > 150000$ yr (Ellington et al. 1987)
$k_{O_3(aq.)} \leq 6 \times 10^{-5}$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 18$ yr at pH 7 (Yao & Haag 1991).

Biodegradation: $t_{1/2}(aq. aerobic) = 168 – 672$ h, based on aerobic river die-away test data (Ludzack et al. 1958; quoted, Howard et al. 1991; Howard et al. 1991)
$\geq 18$ yr at pH 7 (Yao & Haag 1991).

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

Half-Lives in the Environment:
Air: photooxidation $t_{1/2} = 1299 – 12991$ h, based on measured rate constant $k = 3 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993);
atmospheric transformation lifetime was estimated to be $> 5$ d (Kelly et al. 1994).
Surface water: $t_{1/2} = 168 – 672$ h, based on aerobic river die-away test data (Howard et al. 1991);
photooxidation $t_{1/2} = 314 – 12559$ yr, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991); $t_{1/2} \geq 18$ yr for direct reaction with ozone in water at pH 7 and 22°C (Yao & Haag 1991).
Groundwater: $t_{1/2} = 336 – 8640$ 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 16.1.1.1.1

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

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<th>Equation</th>
<th>Log Form</th>
<th>Ln Form</th>
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<td>$P = A - B/(T/K)$</td>
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<td>$P = A - B/(C + t/°C)$</td>
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<td>$P = A - B/(T/K) - C \cdot \log (T/K)$</td>
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<td>$P = A - B/(T/K) - C \cdot \log (T/K)$</td>
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(Continued)
### TABLE 16.1.1.1.1 (Continued)

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<th>T/K</th>
<th>comparative ebulliometry</th>
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<td>eq. 3</td>
<td>P/kPa</td>
<td>t/°C</td>
<td>P/Pa</td>
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<td>P/mmHg</td>
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<td>C</td>
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<td>for temp range 354.5–535 K</td>
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# data not used in regression

**FIGURE 16.1.1.1.1** Logarithm of vapor pressure versus reciprocal temperature for acetonitrile.
TABLE 16.1.1.1.2
Reported Henry’s law constants of acetonitrile at various temperatures and temperature dependence equations

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

Snider & Dawson 1985

<table>
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<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
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<tbody>
<tr>
<td>0</td>
<td>0.614</td>
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<tr>
<td>25</td>
<td>2.066</td>
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</table>

enthalpy of transfer: \( \Delta H/(kJ \cdot mol^{-1}) = 30.54 \)

Benkelberg et al. 1995

<table>
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<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
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<tr>
<td>6</td>
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<td>1.477</td>
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<tr>
<td>20</td>
<td>1.685</td>
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</table>

eq. 3 \( H/atm \)

\( A = 13.8 \pm 0.3 \)

\( B = 4106 \pm 101 \)

FIGURE 16.1.1.1.2 Logarithm of Henry’s law constant versus reciprocal temperature for acetonitrile.
16.1.1.2 Propionitrile

Common Name: Propionitrile
Synonym: propanenitrile, ethyl cyanide, cyanoethane, propyl nitrile
Chemical Name: propionitrile
CAS Registry No: 107-12-0
Molecular Formula: C\(_3\)H\(_5\)N, CH\(_3\)CH\(_2\)CN
Molecular Weight: 55.079
Melting Point (°C): -92.78 (Lide 2003)
Boiling Point (°C): 97.14 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
- 0.7818 (Weast 1982–83; Dean 1985)
- 0.78182, 0.77682 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
- 78.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
- 33.54 (pK\(_a\), Riddick et al. 1986)
Enthalpy of Vaporization, \(\Delta H_{\text{vap}}\) (kJ/mol):
- 37.41, 32.77 (25°C, bp, Dreisbach 1961)
- 36.03, 30.96 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
- 5.045 (Riddick et al. 1986)
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/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):
- 104950 (Seidell 1941)
- 105200 (Hansch et al. 1968)
- 103000 (Dean 1985; Riddick et al. 1986; Howard 1990)
- 55000, 65000 (20°C, 30°C, shake flask-GC, measured range 0–90°C, Stephenson 1994)
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):
- 6005* (interpolated-regression of tabulated data, temp range –35–97.1°C, Stull 1947)
- 10114* (35.5°C, ebulliometry, measured range 35.5–97.35°C, Dreisbach & Shrader 1949)
\[
\log (P/\text{mmHg}) = 7.15217 - 1398.2/(230 + t/°C);\text{ temp range 35.5–97.35°C, (Antoine eq., Dreisbach & Martin 1949)}
\]
- 5333* (22.05°C, measured range –84.66–22.05°C, Milazzo 1956)
- 5950 (calculated by formula, Dreisbach 1961)
\[
\log (P/\text{mmHg}) = 7.05846 - 1327.9/(221.0 + t/°C),\text{ temp range: 17–137°C, (Antoine eq. for liquid state, Dreisbach 1961)}
\]
\[
\log (P/\text{mmHg}) = -0.2185 \times 8769.0/(T/K) + 8.079473;\text{ temp range: –35 to 97.1°C, (Antoine eq., Weast 1972–73)}
\]
- 6140 (22.05°C, quoted exptl., Boublik et al. 1973, 1984)
- 6163, 6143 (extrapolated values-Antoine eq., Boublik et al. 1984)
\[
\log (P/\text{kPa}) = 5.89149 - 1181.562/(160.551 + t/°C),\text{ temp range: 35.5–97.39°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]
\[
\log (P/\text{kPa}) = 4.43918 - 677.415/(160.551 + t/°C),\text{ temp range: –84.7 to 22.05°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]
log (P/mmHg) = 5.2782 – 665.52/(159.0 + t°C), temp range: -84 to 22°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.2770 – 1398.2/(230 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 7.15190 – 1894.10/(T/K); temp range: 9–25°C, (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 33.7908 – 2.9113 × 10^3/(T/K) – 9.1506·log (T/K) + 1.1173 × 10^{-11}·(T/K) + 3.2756 × 10^{-6}·(T/K)^2; temp range 180–564 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
3.800 (partial pressure, Butler & Ramchandani 1935)
3.748 (partial vapor pressure-GC, Buttery et al. 1969)
3.752, 3.752, 4.114 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
5.947 (Howard 1990)

Octanol/Water Partition Coefficient, log K_{OW}:
0.041 (shake flask, Collander 1951)
0.16 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)
– 0.10 (shake flask-GC, Tanii & Hashimoto 1984)
0.16 (recommended, Sangster 1989, 1993)
0.16 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
– 0.108 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:
0.079 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:
Volutilization: using Henry’s law constant, t_1/2 = 13.3 h was estimated for a model river 1 m deep flowing 1 m/s with wind speed 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:
Oxidation: rate constant k, for gas-phase second order reaction 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} = (1.94 ± 0.20) × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298.2 K, measured range 298–423 K (flash photolysis-resonance fluorescence, Harris et al. 1981)
k_{OH} = 1.9 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1985)
k_{OH} = 1.94 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298.2 K, k(soln) = 1.60 × 10^{-13} cm^3 molecule^{-1} s^{-1} for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)
photooxidation t_1/2 = 83 d in air, based on experimental rate constant assuming t_1/2 = 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and t_1/2 > 100 d for the reaction with ozone in the atmosphere (Howard 1990)
k_{OH} = 0.194 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298.2 K (review, Atkinson 1989)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
Half-Lives in the Environment:

Air: $t_{1/2} = 83$ d, based on experimental rate constant assuming 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2} > 100$ d for the reaction with ozone in the atmosphere (Harris et al. 1981; quoted, Howard 1990).

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<th>TABLE 16.1.1.2.1</th>
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FIGURE 16.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propionitrile.
FIGURE 16.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for propionitrile.
16.1.1.3 Butyronitrile

Common Name: n-Butyronitrile
Synonym: butanenitrile
Chemical Name: butyronitrile
CAS Registry No: 109-74-0
Molecular Formula: C₄H₇N, CH₃CH₂CH₂CN
Molecular Weight: 69.106
Melting Point (°C):
   -111.9 (Lide 2003)
Boiling Point (°C):
   117.6 (Lide 2003)
Density (g/cm³):
   0.7911, 0.7865 (20°C, 25°C, Riddick et al. 1986)
Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
   88.4 (30°C, Stephenson & Malanowski 1987)
   100.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
   39.33, 34.43 (25°C, bp, Riddick et al. 1986)
Enthalpy of Sublimation, ∆Hₛᵤ (kJ/mol):
   5.021 (Riddick et al. 1986)
Entropy of Fusion, ∆Sₕᵤ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕᵤ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Other data at other temperatures designated * are compiled at the end of this section):
   33000 (selected, Riddick et al. 1986)
   33500* (20°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1994)
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):
   1333* (25.7°C, summary of literature data, temp range –20 to 117.5°C, Stull 1947)
   3592* (30.64°C, ebulliometry, measured range 30.64–120.223°C, Meyer et al. 1971)
   log (P/mmHg) = 6.771124 – 1444.5851/(t/°C + 223.275); temp range 30.64–120.223°C (Antoine eq., ebulliometric measurements, Meyer et al. 1971)
   2546 (selected, Riddick et al. 1986)
   log (P/kPa) = 6.25390 – 1452.076/(t/°C + 224.1855); temp range not specified (Riddick et al. 1986)
   log (Pₕ/kPa) = 6.25397 – 1452.076/(-46.9645 + T/K); temp range 332–401 K (Antoine eq., Stephenson & Malanowski 1987)
   log (P/mmHg) = 4.8780 – 2.5505 × 10³/(T/K) + 3.6306-log (T/K) – 1.663 × 10⁻²·(T/K) + 1.0604 × 10⁻⁵·(T/K)²; temp range 161–582 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐₒω:
   0.53 (shake flask-GC, Tani & Hashimoto 1984)
   0.53 (recommended, Sangster 1993; Hansch et al. 1995)
Bioconcentration Factor, log BCF or log K_{oc};

Sorption Partition Coefficient, log K_{OC};

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A 6.771124
B 1444.5851
C 223.275
**FIGURE 16.1.1.3.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butyronitrile.

**FIGURE 16.1.1.3.2** Logarithm of vapor pressure versus reciprocal temperature for butyronitrile.
16.1.1.4 Acrylonitrile (2-Propenenitrile)

Common Name: Acrylonitrile
Synonym: cyanoethylene, propenenitrile, 2-propenenitrile, vinyl cyanide
Chemical Name: acrylonitrile, cyanoethylene
CAS Registry No: 107-13-1
Molecular Formula: C₃H₃N, CH₂=CHCN
Molecular Weight: 53.063
Melting Point (°C):
  −83.48 (Lide 2003)
Boiling Point (°C):
  77.30 (Riddick et al. 1986; Howard 1989; Lide 2003)
Density (g/cm³ at 20°C):
  0.8060, 0.8004 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  65.8 (20°C, calculated-density)
  71.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
  Enthalpy of Fusion, ∆Hₚ (kJ/mol):
    6.230 (Riddick et al. 1986)
Entropy of Fusion, ∆Sₚ (J/mol K):
  Fugacity Ratio at 25°C (assuming ∆Sₚ = 56 J/mol K), 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):
  79000 (Klein et al. 1957)
  75000 (Günther et al. 1968)
  73500 (20°C, Windholz 1976)
  73240 (shake flask-LSC, Veith et al. 1980)
  73500 (20°C, Riddick et al. 1986)
  69000*, 66400 (20°C, 30°C, shake flask-GC, measured range 0–70°C, Stephenson 1994)
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):
  14340* (interpolated-regression of tabulated data, temp range −51 to 78.5°C, Stull 1947)
  11732* (20°C, temp range 20–77°C, Gudkov et al. 1964; quoted, Boublik et al. 1984)
  14100 (Hoy 1970)
  log (P/mmHg) = [−0.2185 × 7941.4/(T/K)] + 7.851016; temp range: −51 to 78.5°C, (Antoine eq., Weast 1972–73)
  14720 (extrapolated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 4.77668 – 649.583/(155.006 + t°C), temp range 20–70°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  14370 (Daubert & Danner 1985)
  15240 (calculated-Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 7.03855 – 1232.53/(222.47 + t°C), temp range −20 to 140°C (Antoine eq., Dean 1985, 1992)
  11000 (20°C, Riddick et al. 1986)
  log (P/kPa) = 6.643 – 11644.7/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
  14560 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.12021 – 1288.9/(−38.74 + T/K); temp range 257–352 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.4811 – 1518.381/(−12.003 + T/K); temp range 283–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)
Nitrogen and Sulfur Compounds

\[ \log (P/\text{mmHg}) = 35.921 - 2.7763 \times 10^{3}/(T/K) - 10.101 \log (T/K) - 3.1547 \times 10^{-10}(T/K)^2; \]
\[ \text{temp range 190–535 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 8.918 (calculated-P/C, Mabey et al. 1982)
- 9.420 (quoted, WERL Treatability Database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
- 0.25 (shake flask-HPLC, Pratesi et al. 1979)
- 0.00 (shake flask, Fujisawa & Masuhara 1980, 1981)
- 0.09 (shake flask-GC, Tani & Hashimoto 1984)
- 0.25 (Hansch & Leo 1985)
- 0.25 (recommended, Sangster 1989)
- 0.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{oa} \):

Bioconcentration Factor, log \( BCF \):
- 1.68 (bluegill sunfish, Barrows et al. 1978)
- 0.00 (estimated-S, Kenaga 1980)
- 1.68, 0.32 (bluegill sunfish, calculated-\( K_{ow} \), Veith et al. 1980)
- 0.017 (microorganisms-water, calculated-\( K_{ow} \), Mabey et al. 1982)

Sorption Partition Coefficient, log \( K_{oc} \):
- 0.954 (soil, calculated-S, Kenaga 1980)
- -0.071 (sediment-water, calculated-\( K_{ow} \), Mabey et al. 1982)
- 1.101, 1.006, 1.09 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- -0.0899 (calculated-\( K_{ow} \), Walton et al. 1992)
- -0.0890 (calculated-\( K_{ow} \), Kollig 1993)

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

Volatilization: \( t_{1/2} = 6, 1.2, 4.8 \) d in a typical pond, river and lake are 6, 1.2, and 4.8 d, respectively, with the reaeration for oxygen in typical bodies of water (Lyman et al. 1982; quoted, Howard 1989)
- evaporation \( t_{1/2} = 795 \) min from water with an assumed 1-m depth (Basu et. al. 1983).

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{O3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated, \(^{\text{a}}\)data at other temperatures see reference:
- \( k < 1 \times 10^6 \) M\(^{-1}\) h\(^{-1}\) for singlet oxygen, and 36 M\(^{-1}\) h\(^{-1}\) for peroxy radical at 25°C (Mabey et al. 1982)
- \( t_{1/2} = 4.0 \) h for photooxidation in the troposphere (Callahan et al. 1979)
- \( k_{OH} = (40.6 \pm 4.1) \times 10^{-13} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 299 K (flash photolysis-resonance fluorescence technique, Harris et al. 1981)
- \( k_{O3} < 1 \times 10^{-19} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 296 ± 2 K, and tropospheric lifetimes, \( \tau > 115 \) d and \( \tau = 3 \) d due to reactions with O\(_3\) and OH radical, respectively (Atkinson et al. 1982)
- \( k_{O3} < 1 \times 10^{-19} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 296 ± 2 K (Atkinson et al. 1983; quoted, Atkinson & Carter 1984)
- \( t_{1/2} = 3.5 \) d for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989)
- \( k_{OH} = 4.8 \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 298.7 K, and \( k_{OH} = 3.4 \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 296 K (review, flash photolysis-resonance fluorescence technique Atkinson 1985)
- photooxidation \( t_{1/2} = 3.4–189 \) h, based on measured rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)
- \( k_{OH} = (3.4 – 4.80) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 296–298.2 K (review, Atkinson 1989)
Hydrolysis: \( \text{k(acid)} = 4.2 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1} \) at pH 5.0 with \( t_{1/2} = 188 \text{ yr} \) and \( \text{k(base)} = 6.1 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1} \) at pH 9.0 with \( t_{1/2} = 13 \text{ yr} \) (Ellington et al. 1987; quoted, Howard et al. 1991, Kollig 1993); \( t_{1/2} = 1210 \text{ yr} \) at pH 7.0, based on measured acid and base catalyzed hydrolysis constants (Ellington et al. 1987; quoted, Howard et al. 1991)
\( t_{1/2} = 69 \text{ d} \) at pH 2, \( t_{1/2} = 440000 \text{ d} \) at pH 7 and \( t_{1/2} = 4.7 \text{ d} \) at pH 12 in natural waters (Capel & Larson 1995).

Biodegradation: \( \text{t}_{1/2}(\text{aq. aerobic}) = 30–552 \text{ h} \), based on river die-away test data (Going et al. 1979; Ludzack et al. 1958; quoted, Howard et al. 1991); \( \text{t}_{1/2}(\text{aq. anaerobic}) = 120–2208 \text{ h} \), based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

\( ^{14} \text{C} \) labeled acrylonitrile at concentrations up to 100 ppm was completely degraded within 2.0 d in a London soil under aerobic conditions (Donberg et al. 1992)
\( \text{t}_{1/2}(\text{aerobic}) = 1.3 \text{ d}, \text{t}_{1/2}(\text{anaerobic}) = 5 \text{ d} \) in natural waters (Capel & Larson 1995)

Biotransformation: \( \text{k} = 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1} \) for bacterial transformation in water (Mabey et al. 1982).

**TABLE 16.1.1.4.1**

Reported aqueous solubilities and vapor pressures of acrylonitrile at various temperatures

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Half-Lives in the Environment:

Air: \( \text{t}_{1/2} = 4.0 \text{ h} \) for photooxidation in the troposphere (Callahan et al. 1979);
\( \text{t}_{1/2} = 3.5 \text{ d} \) for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989);
photooxidation \( \text{t}_{1/2} = 13.4–189 \text{ h} \), based on measured rate constant for the reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be \( 1 – 5 \) to > 5 d (Kelly et al. 1994).

Surface water: \( \text{t}_{1/2} = 30–552 \text{ h} \), based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biodegradation \( \text{t}_{1/2}(\text{aq. aerobic}) = 100 \text{ d} \), \( \text{t}_{1/2}(\text{anaerobic}) = 400 \text{ d} \); hydrolysis \( \text{t}_{1/2} = 69 \text{ d} \) at pH 2, \( \text{t}_{1/2} = 440000 \text{ d} \) at pH 7 and \( \text{t}_{1/2} = 4.7 \text{ d} \) at pH 12 in natural waters (Capel & Larson 1995).
Groundwater: \( \text{t}_{1/2} = 60–1104 \text{ h} \) based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: \( \text{t}_{1/2} < 10 \text{ d} \) in soil (USEPA 1979; quoted, Ryan et al. 1988);
\( \text{t}_{1/2} = 30–552 \text{ h} \) based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
FIGURE 16.1.1.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for acrylonitrile.

Acrylonitrile: solubility vs. 1/T

FIGURE 16.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for acrylonitrile.

Acrylonitrile: vapor pressure vs. 1/T
### 16.1.1.5 Benzonitrile

**Chemical Name:** Benzonitrile, benzoic acid nitrile

**CAS Registry No:** 100-47-0

**Molecular Formula:** C₆H₅CN

**Molecular Weight:** 103.122

**Melting Point (°C):**
-13.99 (Lide 2003)

**Boiling Point (°C):**
191.1 (Lide 2003)

**Density (g/cm³ at 20°C):**
- 1.0006 (25°C, Dean 1985; Riddick et al. 1986)

**Molar Volume (cm³/mol):**
- 103.1 (25°C, calculated-density)
- 107.9 (calculated-Le Bas method at normal boiling point)

**Dissociation Constant, pKₐ:**

**Enthalpy of Vaporization, ΔHV (kJ/mol):**
55.48, 45.94 (25°C, bp, Riddick et al. 1986)

**Enthalpy of Fusion, ΔH₅ (kJ/mol):**
- 10.88 (Riddick et al. 1986)

**Entropy of Fusion, ΔS₅ (J/mol K):**

**Fugacity Ratio at 25°C (assuming ΔS₅ = 56 J/mol K), 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):**
- 4330 (shake flask-UV, McGowan et al. 1966)
- 2000 (Dean 1985; Riddick et al. 1986)
- 10000 (selected, Yaws et al. 1990)
- 4000* (shake flask-GC/TC, measured range 0–90°C, Stephenson 1994)

**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, static method, measured range 38.4–190.6°C, Kahlbaum 1898)
- 133.3* (28.2°C, summary of literature data, temp range 28.2–190.6°C, Stull 1947)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**
- 55.32 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

**Octanol/Water Partition Coefficient, log K_{OW}:**

- 1.56 (shake flask-UV spectrophotometry, Fujita et al. 1964; quoted, Leo et al. 1969; Hansch & Leo 1979)
- 1.56 (shake flask-UV, Holmes & Lough 1976)
Nitrogen and Sulfur Compounds

1.67  (calculated-fragment const., Rekker 1977)
1.56  (shake flask at pH 7, Unger et al. 1978)
1.66  (RP-HPLC-k' correlation, Miyake & Terada 1982)
1.65 ± 0.01  (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.50  (HPLC-k' correlation, Haky & Young 1984)
1.56  (shake flask-GC, Tanii & Hashimoto 1984)
1.56  (RP-HPLC-capacity ratio, Minick et al. 1988)
1.45  (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.56  (recommended, Sangster 1989, 1993)
1.56  (shake flask-GC, Alcorn et al. 1993)
1.56  (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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} = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} (Zetisch 1982; Atkinson 1989)
k_{OH}(calc) = 4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} (Atkinson 1985)
k_{OH}(calc) = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} (Atkinson et al. 1985)
k_{OH}(calc) = 3.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{, k}_{OH}(obs) = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} (SAR structure-activity relationship, Atkinson 1987)
k_{OH}(calc) = 4.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Surface water: an estimated t_{1/2} = 1.3 d in Rhine River in case of first order reduction process (Zoeteman et al. 1980)

<table>
<thead>
<tr>
<th>Table 16.1.1.5.1</th>
<th>Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aqueous solubility</strong></td>
<td><strong>Vapor pressure</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Stephenson 1994</strong></td>
</tr>
<tr>
<td></td>
<td><strong>shake flask-GC</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m^{-3}</td>
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<tr>
<td>0</td>
<td>3500</td>
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<tr>
<td>10</td>
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<td>50</td>
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<td>4200</td>
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(Continued)
### TABLE 16.1.1.5.1 (Continued)

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<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
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<tbody>
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<td>Stephenson 1994</td>
<td>Stull 1947</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>
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<tr>
<td>70</td>
<td>6000</td>
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<tr>
<td>80</td>
<td>9500</td>
</tr>
<tr>
<td>90</td>
<td>9100</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>ΔH_{sol}/(kJ mol⁻¹)</td>
<td>113.7</td>
</tr>
<tr>
<td>25 °C</td>
<td>121.3</td>
</tr>
</tbody>
</table>

| Meyer et al. 1971 | Meyer & Hotz 1976 |
| ebulliometry      | ebulliometry      |
| t/°C    | P/Pa | t/°C | P/Pa | t/°C | P/Pa |
| 103.9   | 6666.1 |        |      | 123.5 | 13332 |

**FIGURE 16.1.1.5.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzonitrile.
FIGURE 16.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for benzonitrile.

Benzonitrile: vapor pressure vs. 1/T

$\log(P/\text{Pa})$

$1/(T/\text{K})$

b.p. = 191.1 °C
m.p. = -13.99 °C
16.1.2 ALIPHATIC AMINES

16.1.2.1 Dimethylamine

\[ \begin{array}{c}
\text{H} \\
\text{N}
\end{array} \]

Common Name: Dimethylamine
Synonym: aminomethylmethane, N-methylmethanamine
Chemical Name: aminomethylmethane, dimethylamine
CAS Registry No: 124-40-3
Molecular Formula: C₂H₇N, CH₃NHCH₃
Molecular Weight: 45.084
Melting Point (°C): 
-92.18 (Lide 2003)
Boiling Point (°C): 
6.88 (Lide 2003)
Density (g/cm³ at 20°C): 
0.6804 (0°C, Weast 1982–83)
0.6556, 0.6496 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol): 
68.8 (20°C, calculated-density)
67.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ: 
10.732 (Perrin 1965; Weast 1982–83; Howard 1990)
10.77 (protonated cation + 1, Dean 1985)
10.77 (Sangster 1989)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol): 
23.84, 24.61 (25°C, bp, Dreisbach 1961)
23.65, 24.61 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol): 
5.941 (Riddick et al. 1986)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
very soluble (Dean 1985)
620000 (selected, Yaws et al. 1990)
miscible (Stephenson 1993b)
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):
101141* (280.018 K, static method, measured range 201.387–280.018 K, Ashton et al. 1939)
236420* (extrapolated-regression of tabulated data, temp range –87.2 to + 7.4°C, Stull 1947)
196800 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.06396 – 1024.4/(238.0 + t°C), temp range –55 to 37°C, (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 6660.0/(T/K)] + 7.995166; temp range –87.7 to 162.6°C, (Antoine eq., Weast 1972–73)
172220 (20°C, Verschueren 1983)
206180 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.21132 – 962.001/(221.852 + t°C), temp range –71.77 to 6.858°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
202620 (Daubert & Danne 1985)
206000 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.08212 – 960.242/(221.67 + t°C), temp range –72 to 6°C (Antoine eq., Dean 1985, 1992)
Nitrogen and Sulfur Compounds

196800 (quoted lit., Riddick et al. 1986)
\[ \log (P/kPa) = 6.18886 - 1.024.40/(238.0 + T/°C), \text{ temp range not specified (Antoine eq., Riddick et al. 1986)} \]

205300 (interpolated-Antoine eq.-II., Stephenson & Malanowski 1987)
\[ \log (P/kPa) = 6.29031 - 993.586/(–48.12 + T/K), \text{ temp range 201–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

205300 (quoted lit., Riddick et al. 1986)
\[ \log (P/kPa) = 6.29031 - 993.586/(–48.12 + T/K), \text{ temp range 201–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log (P/kPa) = 7.81489 - 2369.425/(141.433 + T/K), \text{ temp range 358–438 K (Antoine eq.-III, Stephenson & Malanowski 1987)} \]

\[ \log (P/mmHg) = 36.9182 - 2.4965 \times 10^3/(T/K) - 10.417 \cdot \log (T/K) - 1.6287 \times 10^{-9} \cdot (T/K)^2; \text{ temp range 181–438 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 1.796 (exptl., Hine & Mookerjee 1975; quoted, Howard 1990)
- 1.796, 1.03 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 2.718 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- –0.38 (shake flask-RC at pH 13, Wolfenden 1978)
- –0.38 (Hansch & Leo 1985)
- –0.38 (recommended, Sangster 1989; 1993)
- –0.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
- 2.00 (calculated-\( S_{oct} \) and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
- –0.523 (calculated-\( K_{OW} \), Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log \( K_{OC} \):
- 2.638 (adsorption isotherm average for five soils, Rao & Davidson 1982; quoted, Howard 1990)
- 0.602; 2.212; 2.706 (Podzol soil; Alfsisol soil; sediment, von Oepen et al. 1991)
- 2.63 (soil, calculated-MCI, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, \( t_1/2 \):

Volatileization: using Henry’s law constant, \( t_1/2 = 35.1 \text{ h} \) was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; selected, 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 NO₃ radical and \( k_{O_3} \) with O₃ as or as indicated:
  \[ k_{OH} = 6.54 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \text{ K} \text{ (Atkinson et al. 1977; quoted, Carlier et al. 1986; Atkinson 1989)} \]
  \[ \text{photooxidation } t_1/2 = 5.9 \text{ h} \text{ in air was estimated for the vapor phase reaction with hydroxyl radical of } 5 \times 10^5 \text{ radicals/cm}^3 \text{ in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990)} \]
  \[ k_{O_3} = (2.61 \pm 0.30) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K} \text{ (Atkinson & Carter 1984; quoted, Atkinson 1985)} \]
  \[ k_{OH} = 6.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the gas-phase reaction with } 5 \times 10^5 \text{ OH radicals/cm}^3 \text{ at room temp. having a loss rate of } 2.8 \text{ d}^{-1} \text{ (Atkinson 1985)} \]
  \[ k_{OH(calc)} = 63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1987).} \]

Hydrolysis:
- Biodegradation: aqueous aerobic \( t_1/2 = 2–79 \text{ h} \), based on river die-away test data (Digeronimo et al. 1979; Dojlido 1979; selected, Howard et al. 1991); aqueous anaerobic \( t_1/2 = 8–316 \text{ h} \), 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: $t_{1/2} = 5.9$ h was estimated for the vapor phase reaction with hydroxyl radical of $5 \times 10^5$ radicals/cm$^3$ in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

photooxidation $t_{1/2} = 0.892–9.20$ h, based on measured rate constant for the gas-phase reaction with OH radical (Atkinson 1985; quoted, Howard et al. 1991) and ozone (Tuazon et al. 1978; selected, Howard et al. 1991).

Surface water: $t_{1/2} = 2–79$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 4–158$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:


Biota:

<table>
<thead>
<tr>
<th>TABLE 16.1.2.1.1</th>
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</thead>
<tbody>
<tr>
<td>Reported vapor pressures of dimethylamine at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

\[
\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/(C + T/K - C\log (T/K)) \\
\log P &= A - B/(C + T/K - C\log (T/K) + D\cdot(T/K) - E\cdot(T/K)^2 + F\cdot(T/K)^3)
\end{align*}

Ashton et al. 1939  \hspace{1cm} Stull 1947

<table>
<thead>
<tr>
<th>$T/K$</th>
<th>$P$/Pa</th>
<th>static method</th>
<th>$t/°C$</th>
<th>$P$/Pa</th>
<th>summary of literature data</th>
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<tr>
<td>201.387</td>
<td>648</td>
<td>bp/K</td>
<td>280.04</td>
<td>–87.7</td>
<td>133.3</td>
</tr>
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<td>213.802</td>
<td>1959</td>
<td>mp/K</td>
<td>180.97</td>
<td>–72.2</td>
<td>666.6</td>
</tr>
<tr>
<td>222.078</td>
<td>3780</td>
<td>\Delta H_{fus}/(kJ mol^{-1}) = 26.48 (bp)</td>
<td>–64.6</td>
<td>1333</td>
<td></td>
</tr>
<tr>
<td>232.137</td>
<td>7775</td>
<td>\Delta H_{fus}/(kJ mol^{-1}) = 5.94 (mp)</td>
<td>–56.0</td>
<td>2666</td>
<td></td>
</tr>
<tr>
<td>242.078</td>
<td>14743</td>
<td>\Delta H_{fus}/(kJ mol^{-1}) = 26.48 (bp)</td>
<td>–46.7</td>
<td>5333</td>
<td></td>
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<tr>
<td>249.640</td>
<td>8460</td>
<td>eq. 5</td>
<td>P/mmHg</td>
<td>–40.7</td>
<td>7999</td>
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<td>256.449</td>
<td>33269</td>
<td>A</td>
<td>32.26370</td>
<td>–32.6</td>
<td>13332</td>
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<tr>
<td>262.977</td>
<td>46404</td>
<td>B</td>
<td>2460.10</td>
<td>–20.4</td>
<td>26664</td>
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<tr>
<td>270.182</td>
<td>65491</td>
<td>C</td>
<td>8.6390</td>
<td>–7.1</td>
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<tr>
<td>275.934</td>
<td>84860</td>
<td>D</td>
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<td>7.4</td>
<td>101325</td>
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<tr>
<td>279.980</td>
<td>100974</td>
<td>E</td>
<td>3.51389×10^{-5}</td>
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<tr>
<td>277.680</td>
<td>91519</td>
<td>F</td>
<td>5.3241×10^{-8}</td>
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<tr>
<td>280.018</td>
<td>101141</td>
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</table>

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FIGURE 16.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethylamine.
16.1.2.2 Trimethylamine

Common Name: Trimethylamine
Synonym: dimethylamino methane, TMA
Chemical Name: trimethylamine
CAS Registry No: 75-50-3
Molecular Formula: C₃H₉N, CH₃N(CH₃)₂
Molecular Weight: 59.110
Boiling Point (°C): 2.87 (Lide 2003)
Density (g/cm³ at 20°C): 0.6356 (Weast 1982–83)
Molar Volume (cm³/mol):
93 (20°C, calculated-density)
93.3 (calculated-Le Bas method at normal boiling point)
9.80 (pKₐ, protonated cation + 1, Dean 1985)
9.79 (pKₐ, Sangster 1989)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
22.85, 24.13 (25°C, bp, Dreisbach 1961)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C) or as indicated:
410000 (Dean 1985)
890000 (30°C, Howard 1990)
291000 (selected, Yaws et al. 1990)
miscible (Stephenson 1993b)
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 chapter):
221715* (isoteniscope, measured range 0–40°C, Swift & Hochanadel 1945)
log (P/mmHg) = 24.91300 – 2018.37/(T/K) – 6.0303 · log (T/K); temp range 0–40°C (isoteniscope method, Swift & Hochanadel 1945)
265200* (extrapolated-regression of tabulated data, temp range −97.1 to + 2.9°C, Stull 1947)
226540 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 6.97038 – 968.7/(234.0 + t°C), temp range −58 to 32°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [−0.2185 × 6361.7/(T/K)] + 7.952370; temp range −97.1 to 2.9°C (Antoine eq., Weast 1972–73)
192500 (20°C, 30°C, Verschueren 1983)
192500 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.87712 – 894.366/(228.276 + t°C), temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
219300, 221800 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.85755 – 955.94/(237.52 + t°C), temp range −80 to 3°C (Antoine eq., Dean 1985, 1992)
219900 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log \( \frac{P}{kPa} \) = 6.01402 – 968.978/(-34.253 + T/K), temp range 192–277 K (Antoine eq., Stephenson & Malanowski 1987)

log \( \frac{P}{mmHg} \) = 58.6807 – 2.686 \times 10^3/(T/K) – 20.36\log (T/K) + 1.3131 \times 10^{-2} \cdot (T/K) – 6.563 \times 10^{-13} \cdot (T/K)^2; temp range 156–433 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 6.672 (exptl., Hine & Mookerjee 1975)
- 12.71, 2.16 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 15.64 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- 0.27 (shake flask-TN, Sandell 1962; quoted, Leo et al. 1971)
- 0.27; 0.20 (calculated-f const., calculated-\( \pi \) const., Rekker 1977)
- 0.16 (shake flask, Hansch & Leo 1985)
- 0.16 (recommended, Sangster 1989)
- 0.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
- Bioconcentration Factor, log \( BCF \):
  - < 0.0 (estimated-\( K_{OW} \), Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log \( K_{OC} \):
- 1.462 (soil, estimated-\( K_{OW} \), Lyman et al. 1982; quoted, Howard 1990)
- 0.602 (soil, estimated-solubility, Lyman et al. 1982; quoted, Howard 1990)
- 0.778; 2.365; 2.831 (Podzol soil; Alfisol soil; sediments von Oepen et al. 1991)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\frac{1}{2} \):
- Volatilization: using Henry’s law constant, \( t_\frac{1}{2} = 11 \) h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).
- 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:
  - \( k_{OH} = 6.09 \times 10^{-11} \) cm³ molecule⁻¹ s⁻¹ at 299 K (Atkinson et al. 1977; Atkinson 1989)
  - photooxidation \( t_\frac{1}{2} = 62 \) d in water, based on rate constant \( k = 1.3 \times 10^{10} \) L mol⁻¹ s⁻¹ for the reaction with photochemically produced hydroxyl radicals of \( 1 \times 10^{-17} \) mol · L⁻¹ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)
  - \( k_{OH} = 6.10 \times 10^{-11} \) cm³ molecule⁻¹ s⁻¹ for the gas-phase reaction with \( 1 \times 10^6 \) OH radicals/cm³ with a loss rate of \( 5.0 \) d⁻¹ and rate constant \( k_{O3} = 9.70 \times 10^{-18} \) cm³ molecule⁻¹ s⁻¹ for the gas-phase reaction with \( 7 \times 10^{11} \) O₃ molecules/cm³ with a loss rate of \( 0.6 \) d⁻¹ both at room temp. (Atkinson & Carter 1984)
  - calculated \( k_{OH} = 64 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987).
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
- Air: photodestruction \( t_\frac{1}{2} = 4.0 \) h, based on rate constant \( k = 6.09 \times 10^{-11} \) cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radical of \( 8 \times 10^5 \) radicals/cm³ in air at 25.5°C and \( t_\frac{1}{2} = 1.4 \) d, based on rate constant \( k = 9.73 \times 10^{-10} \) cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with ozone of \( 6 \times 10^{11} \) molecules/cm³ in air at 24.4°C (Atkinson 1985; GEMS 1986; quoted, Howard 1990).
- Surface water: \( t_\frac{1}{2} = 62 \) d, based on rate constant \( k = 1.3 \times 10^{10} \) L mol⁻¹ s⁻¹ for the reaction with photochemically produced hydroxyl radicals of \( 1 \times 10^{-17} \) mol L⁻¹ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).
TABLE 16.1.2.2.1
Reported vapor pressures of trimethylamine at various temperatures and the coefficients for the vapor pressure equations

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

Aston et al. 1944
Swift & Hochanadel 1945
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>–80.315</td>
<td>805</td>
<td>0</td>
<td>91059</td>
<td>–97.1</td>
<td>133.3</td>
</tr>
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<td>–74.081</td>
<td>1367</td>
<td>15</td>
<td>158520</td>
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<td>666.6</td>
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<td>3354</td>
<td>20</td>
<td>188651</td>
<td>–73.8</td>
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<td>–51.938</td>
<td>6777</td>
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<tr>
<td>–46.842</td>
<td>9305</td>
<td>30</td>
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<td>40</td>
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<td>221715</td>
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<tr>
<td>–24.155</td>
<td>31772</td>
<td>bp/K</td>
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<td>–12.5</td>
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<td>–20.164</td>
<td>38401</td>
<td>eq. 4</td>
<td>P/mmHg</td>
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<td>–15.974</td>
<td>46505</td>
<td>A</td>
<td>24.91300</td>
<td>mp/°C</td>
<td>–117.1</td>
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<td>–11.422</td>
<td>56802</td>
<td>B</td>
<td>2018.37</td>
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<td>–8.985</td>
<td>63039</td>
<td>C</td>
<td>6.0303</td>
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<td>–7.399</td>
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<td>–3.113</td>
<td>80208</td>
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<td></td>
<td>ΔH_v/(kJ mol⁻¹) = 23.93</td>
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</tr>
<tr>
<td>0.780</td>
<td>93495</td>
<td>at bp</td>
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</tr>
</tbody>
</table>

FIGURE 16.1.2.2.1 Logarithm of vapor pressure versus reciprocal temperature for trimethylamine.
16.1.2.3 Ethylamine

Common Name: Ethylamine
Synonym: aminoethane, ethanamine, monoethylamine
Chemical Name: aminoethane, ethylamine
CAS Registry No: 75-04-7
Molecular Formula: C₂H₇N, CH₃CH₂NH₂
Molecular Weight: 45.084

Melting Point (°C):
-80.5 (Lide 2003)

Boiling Point (°C):
16.5 (Lide 2003)

Density (g/cm³ at 20°C):
0.6829 (Dreisbach 1961; Weast 1982–83)
0.6769 (25°C, Dreisbach 1961)

Molar Volume (cm³/mol):
65.4 (5°C, Stephenson & Malanowski 1987)
66.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
10.79 (Perrin 1972)
10.81 (20°C, Weast 1982–83)
10.63 (protonated cation + 1, Dean 1985)
10.70 (Sangster 1989)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
27.08, 27.57 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔHₕ (kJ/mol):
Entropy of Fusion, ΔSₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕ = 56 J/mol K), F: 1.0

Water Solubility (g/mL at 25°C):
miscible (Dean 1985; Howard 1990; Stephenson 1993b)

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):
156200* (extrapolated-regression of tabulated data, temp range –82.3 to 16.6°C, Stull 1947)
141620 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.3862 – 1137.30/(235.85 + t°C); temp range –43 to 47°C (Antoine eq. for liquid state, Dreisbach 1961)
93325* (20°C, temp range 1.95 to 20°C, Bittrich et al. 1962)
log (P/mmHg) = [–0.2185 × 6845.1/(T/K)] + 7.973674; temp range –82.3 to 176°C, (Antoine eq., Weast 1972–73)
121570, 172220 (20°C, 30°C, Verschueren 1983)
139100 (extrapolated-Antoine eq., Boulik et al. 1984)
log (P/kPa) = 5.12561 – 559.427/(162.579 + t°C); temp range 1.95–14.65°C (Antoine eq. from reported exptl. data, Boulik et al. 1984)
139700 (Daubert & Danner 1985)
141000 (calculated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.05413 – 987.31/(220.00 + t°C); temp range –20 to 90°C (Antoine eq., Dean 1985, 1992)
137500, 141200 (calculated-Antoine eq.-II, III, Stephenson & Malanowski 1987)
log (P/kPa) = 6.57462 – 1167.57/(34.18 + T/K); temp range 213–297 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.43082 – 1140.62/(–32.433 + T/K); temp range 290–449 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_l/kPa) = 6.21526 – 1009.66/(–49.804 + T/K); temp range 291–367 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_l/kPa) = 6.48782 – 1176.995/(–26.674 + T/K); temp range 377–456 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

140900 (calculated-Cox eq., Chao et al. 1990)

log (P/mmHg) = 33.2962 – 2.4307 × 103/(T/K) – 9.0779·log (T/K) – 1.3848 × 10–9·(T/K) + 3.8183 × 10–6·(T/K)²; temp range 192–456 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
1.012 (partial pressure, Butler & Ramchandani 1935)
0.683 (exptl., Hine & Mookerjee 1975)
0.859, 0.730 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.421 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.30 (shake flask-titration with ion correction, Korenman et al. 1973)
–0.16, –0.14; –0.19 (calculated-fragment const.; calculated-π const., Rekker 1977)
–0.13 (Hansch & Leo 1985)
–0.13 (recommended, Sangster 1989)
–0.14 (calculated-CLOGP, Jäckel & Klein 1991)
–0.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
< 0.0 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: using Henry’s law constant, t½ = 2.0 d was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1990).
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:
photooxidation t½ > 9.9 d for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

k_{OH} = 2.77 × 10–11 cm³·molecules–1·s–1 at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986)
photooxidation t½ = 321 d in water, based on rate constant k = 2.5 × 10⁹ L·mol⁻¹·s⁻¹ for the aqueous-phase reaction with photochemically produced OH radical of 1 × 10⁻¹⁷ mol·L⁻¹ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

k_{O3} = (2.76 ± 0.34) × 10⁻²⁰ cm³·molecules⁻¹·s⁻¹ at 296 ± 2 K under atmospheric conditions (Atkinson & Carter 1984)

k_{OH} = 27.7 × 10⁻¹² cm³·molecule⁻¹·s⁻¹ at 299.6 K (Atkinson 1989)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:
Air: t½ > 9.9 d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
photooxidation t½ = 8.6 h, based on rate constant k = 6.54 × 10⁻¹¹ cm³·molecules⁻¹·s⁻¹ for the vapor-phase reaction with an average hydroxyl radical of 5 × 10⁵ radicals/cm³ at 25.5°C (Atkinson 1985; quoted, Howard 1990).
Surface water: $t_{1/2} = 321$ d, based on a rate constant $k = 2.5 \times 10^9$ L·mol$^{-1}$·s$^{-1}$ for the aqueous-phase reaction with photochemically produced hydroxyl radical of $1 \times 10^{-17}$ mol·L$^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

### TABLE 16.1.2.3.1
Reported vapor pressures of ethylamine at various temperatures

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Bittrich et al. 1962</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$P$/Pa</td>
</tr>
<tr>
<td>–82.3</td>
<td>133.3</td>
</tr>
<tr>
<td>–66.4</td>
<td>666.6</td>
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<tr>
<td>–58.3</td>
<td>1333</td>
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<tr>
<td>–48.6</td>
<td>2666</td>
</tr>
<tr>
<td>–39.8</td>
<td>5333</td>
</tr>
<tr>
<td>–33.4</td>
<td>7999</td>
</tr>
<tr>
<td>–25.1</td>
<td>13332</td>
</tr>
<tr>
<td>–12.3</td>
<td>26664</td>
</tr>
<tr>
<td>2.0</td>
<td>53329</td>
</tr>
<tr>
<td>16.6</td>
<td>101325</td>
</tr>
</tbody>
</table>

$\text{mp}/°C = –80.6$

**FIGURE 16.1.2.3.1** Logarithm of vapor pressure versus reciprocal temperature for ethylamine.
16.1.2.4 Diethylamine

Common Name: Diethylamine
Synonym: aminoethylethane, N-ethylethanamine
Chemical Name: aminoethylethane, diethylamine
CAS Registry No: 109-89-7
Molecular Formula: C₄H₁₁N, CH₃CH₂NHCH₂CH₃
Molecular Weight: 73.137
Melting Point (°C):
-49.8 (Lide 2003)
Boiling Point (°C):
55.5 (Lide 2003)
Density (g/cm³ at 20°C):
0.6993, 0.6926 (20°C, 25°C, Dreisbach. 1961)
0.7056 (Weast 1982–83)
0.7070, 0.7016 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
103.4 (20°C, calculated-density)
109.0 (exptl. at normal bp, Lee et al. 1972)
111.9 (calculated-Le Bas method at normal boiling point,)
Dissociation Constant, pKₐ:
10.98 (Perrin 1965; quoted, Howard 1990)
10.80 (35°C, Perrin 1972)
10.80 (protonated cation + 1, Dean 1985)
11.07 (Sangster 1989)
Enthalpy of Vaporization, ∆HV (kJ/mol):
31.38, 29.50 (25°C, bp, Dreisbach 1961)
31.32, 29.07 (25°C, bp, Riddick et al. 1986)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
815000 (14°C, quoted, Verschueren 1983)
miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990)
miscible (Stephenson 1993b)
Vapor Pressure (Pa at 25°C and or as indicated reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):
26664* (21°C, summary of literature data, temp range –33.0 to 55.5°C, Stull 1947)
31130 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.14099 – 1209.9/(229.0 + t°C); temp range –15 to 90°C (Antoine eq. for liquid state, Dreisbach 1961)
39997* (31.45°C, temp range 31.45–60.58°C, Bittrich & Kauer 1962)
31471* (25.17°C, temp range 19.73–40.22°C, Kilian & Bittrich 1965)
log (P/mmHg) = [–0.2185 x 7307.5/(T/K)] + 7.701718; temp range –33.0 to 210°C (Antoine eq., Weast 1972–73)
26660, 38660 (20°C, 30°C, Verschueren 1983)
30110, 31310 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 4.97981 – 580.448/(143.68 + t°C); temp range 31.45–60.58°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.84728 – 994.478/(203.53 + t°C); temp range 19.758–40.22°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
Nitrogen and Sulfur Compounds

(log P/kPa) = 4.92649 – 583.297/(144.145 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

(log P/kPa) = 5.96802 – 1058.538/(–61.331 + T/K); temp range 302–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)

(log P/kPa) = 5.96802 – 1058.538/(–61.331 + T/K); temp range 302–328 K (Antoine eq.-II, Stephenson & Malanowski 1987)

(log P/mmHg) = 5.8016 – 583.3/(144.1 + t/°C); temp range 31–61°C (Antoine eq., Dean 1992)

(log P/mmHg) = 5.8016 – 583.3/(144.1 + t/°C); temp range 31–61°C (Antoine eq., Dean 1992)

Henry’s Law Constant (Pa·m³/mol at 25°C):
2.596 (exptl., Hine & Mookerjee 1975)
2.537, 2.37 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
6.67 (calculated-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:
0.43 (shake flask, Collander 1951)
0.57 (shake flask-titration, Sandell 1962)
0.60, 0.61; 0.70 (calculated-fragment const.; calculated-π const., Rekker 1977)
0.58 (Hansch & Leo 1985)
0.58 (20°C, shake flask-OC, Takayama et al. 1985)
0.81 (HPLC-k′ correlation, Eadsforth 1986)
0.58 (recommended, Sangster 1989)
0.58 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:
0.210 (calculated-K_{ow}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{oc}:
1.699 (soil, calculated-K_{ow}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, τ_{1/2}:
Volatilization: using Henry’s law constant, τ_{1/2} = 31.6 h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Oxidation: photooxidation τ_{1/2} > 9.9 d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976); photooxidation τ_{1/2} = 0.21 d in air, based on an estimated second-order rate constant k = 77.1 × 10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5 × 10⁵ radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_{i}) and Elimination (k_{e}) Rate Constants:

Half-Lives in the Environment:
Air: τ_{1/2} > 9.9 d for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); τ_{1/2} = 0.21 d, based on an estimated rate constant k = 77.1 × 10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5 × 10⁵ radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).
TABLE 16.1.2.4.1
Reported vapor pressures of diethylamine at various temperatures

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Bittrich &amp; Kauer 1962</th>
<th>Kilian &amp; Bittrich 1965</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>–33.0</td>
<td>1333</td>
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<td>51.10</td>
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<tr>
<td>mp/°C</td>
<td>–38.9</td>
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</tr>
</tbody>
</table>

b.p. = 55.5 °C
m.p. = -49.8 °C

FIGURE 16.1.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for diethylamine.
16.1.2.5  \textit{n}-Propylamine

\begin{equation*}
\text{NH}_2
\end{equation*}

Common Name: Propylamine
Synonym: 1-aminopropane, 1-propanamine, \textit{n}-propylamine
Chemical Name: aminopropane, \textit{n}-propylamine
CAS Registry No: 107-10-8
Molecular Formula: C\textsubscript{3}H\textsubscript{9}N, CH\textsubscript{3}CH\textsubscript{2}CH\textsubscript{2}NH\textsubscript{2}
Molecular Weight: 59.110
Melting Point (°C): 
\begin{align*}
-84.75 & \quad \text{(Lide 2003)}
\end{align*}
Boiling Point (°C): 
\begin{align*}
47.22 & \quad \text{(Lide 2003)}
\end{align*}
Density (g/cm\textsuperscript{3} at 20°C): 
\begin{align*}
0.7173 & \quad \text{(Dreisbach 1961; Weast 1982–83; Dean 1985; Riddick et al. 1986)}
0.7123 & \quad \text{(25°C, Dreisbach 1961)}
\end{align*}
Molar Volume (cm\textsuperscript{3}/mol): 
\begin{align*}
82.4 & \quad \text{(liquid molar volume, Kamlet et al. 1986, 1987)}
88.2 & \quad \text{(calculated-Le Bas method at normal boiling point)}
\end{align*}
Dissociation Constant, pK:\n\begin{align*}
10.74, 10.789 & \quad \text{(20°C, Perrin 1972)}
10.71 & \quad \text{(pK\textsubscript{a}, 20°C, Weast 1982–83)}
10.57 & \quad \text{(pK\textsubscript{BH} + , Dean 1985; Riddick et al. 1986)}
10.68 & \quad \text{(pK\textsubscript{a}, Sangster 1989)}
\end{align*}
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol): 
\begin{align*}
31.13, 29.73 & \quad \text{(25°C, bp, Dreisbach 1961)}
31.26, 29.54 & \quad \text{(25°C, bp, Riddick et al. 1986)}
\end{align*}
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol): 
\begin{align*}
10.974 & \quad \text{(Riddick et al. 1986)}
\end{align*}
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K): 
\begin{align*}
\text{Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0}
\end{align*}
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
\begin{align*}
\text{miscible (Dean 1985; Stephenson 1993b)}
\text{miscible (Riddick et al. 1986; Howard 1990; Yaws et al. 1990)}
\end{align*}
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):
\begin{align*}
41800^* & \quad \text{(interpolated-regression of tabulated data, temp range \textendash 64.4 to 48.5°C, Stull 1947)}
41050 & \quad \text{(calculated by formula, Dreisbach 1961)}
\log (P/mmHg) = 7.2672 – 1218.1/(229.9 + t/°C); temp range \textendash 20 to 81°C (Antoine eq. for liquid state, Dreisbach 1961)}
\end{align*}
\begin{align*}
42100^* & \quad \text{(ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)}
\log (P/mmHg) = 6.92640 – 1044.028/(t/°C + 210.833); temp range 23–77.6°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)}
\log ([P/atm] = [1 – 320.379 ± (T/K)] 
\times 10^6[0.922208 – 10.51259 
\times 10^{-3} (T/K) + 11.25530 \times 10^{-7} (T/K)^2); temp range: 34–77.6°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)}
\log (P/mmHg) = [-0.2185 \times 7408.0/(T/K)] + 7.867998; temp range \textendash 64.4 to 214.5°C (Antoine eq., Weast 1972–73)}
32660 & \quad \text{(20°C, 31°C, Verschueren 1983)}
38550; 42110 (22.97°C, quoted expltl., calculated-Antoine eq., Boublik et al. 1984)}
\log (P/kPa) = 6.05146 – 1044.082/(210.84 + t/°C); temp range 22.97–77.6°C (Antoine eq. from reported expltl. data of Osborn & Douslin 1968, Boublik et al. 1984)}
42120 & \quad \text{(calculated-Antoine eq., Dean 1985, 1992)}
\end{align*}
log (P/mmHg) = 6.92651 – 1044.05/(210.84 + t°C); temp range: 23–77°C (Antoine eq., Dean 1985, 1992)

41050 (Riddick et al. 1986)

log (P/kPa) = 6.05136 – 1044.028/(210.833 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

42120 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 24.6420 – 2.3152 × 10^{-3}/(T/K) – 5.8711·log (T/K) – 4.6258 × 10^{-11}/(T/K) + 1.582 × 10^{-6}·(T/K)^2;
temp range 190–497 (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

1.274 (partial pressure, Butler & Ramchandani 1935)

0.784; 0.732 (exptl.; calculated-group contribution, Hine & Mookerjee 1975)

1.330 (calculated-bond contribution, Hine & Mookerjee 1975)

0.637 (calculated-molecular structure, Russell et al. 1992)

2.01 (gas stripping-GC, Altschuh et al. 1999)

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

0.28 (shake flask-GC, Korenman et al. 1973)

0.37, 0.39; 0.31 (calculated-f const.; calculated-π const., Rekker 1977)

0.48 (shake flask-GC, pH 13, Yakayama et al. 1985)

0.48 (recommended, Sangster 1989)

0.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

−0.886 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

< 1.699 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization: using Henry’s law constant, t_{1/2} ~ 2.44 d was estimated for a model river 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation t_{1/2} = 12 h in air, based on estimated rate constant k = 3.21 × 10^{-12} cm^3·molecule^{-1}·s^{-1}

for the vapor-phase reaction with hydroxyl radical of 5 × 10^5/cm^3 at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:

Half-Lives in the Environment:

Air: t_{1/2} = 12 h, based on estimated second-order rate constant of 3.21 × 10^{-12} cm^3·molecule^{-1}·s^{-1} for the vapor-phase reaction with hydroxyl radical of 5 × 10^5/cm^3 at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).
<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
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<tbody>
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<td>27.750</td>
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<td>47.229</td>
<td>101325</td>
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<td>mp/°C</td>
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**FIGURE 16.1.2.5.1** Logarithm of vapor pressure versus reciprocal temperature for n-propylamine.
16.1.2.6  \textit{n}-Butylamine

\begin{center}
\begin{tikzpicture}
\draw (-0.5,0) -- (0.5,0);
\draw (0,-0.5) -- (0,0.5);
\end{tikzpicture}
\end{center}

Common Name: Butylamine
Synonym: 1-aminobutane, \textit{n}-butylamine, 1-butanamine
Chemical Name: 1-aminobutane, \textit{n}-butylamine
CAS Registry No: 109-73-9
Molecular Formula: \text{C}_4\text{H}_{11}\text{N}, \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2
Molecular Weight: 73.137
Melting Point (°C):
\begin{itemize}
  \item –49.1 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
\end{itemize}
Boiling Point (°C):
\begin{itemize}
  \item 77.0 (Lide 2003)
\end{itemize}
Density (g/cm$^3$ at 20°C):
\begin{itemize}
  \item 0.7414 (Dreisbach 1961; Weast 1982–83)
  \item 0.7392 (Riddick et al. 1986)
\end{itemize}
Molar Volume (cm$^3$/mol):
\begin{itemize}
  \item 98.8 (20°C, calculated-density)
  \item 110.4 (calculated-Le Bas method at normal boiling point)
\end{itemize}
Dissociation Constant, pK:
\begin{itemize}
  \item 10.77 (Perrin 1965; pK$_{a}$, 20°C, Weast 1982–83; Howard 1990)
  \item 10.65 (Perrin 1972)
  \item 10.64 (pK$_{a}$ protonated + 1, Dean 1985; Sangster 1989)
  \item 10.77 (pK$^{B+}$, Riddick et al. 1986)
\end{itemize}
Enthalpy of Vaporization, $\Delta H_{v}$ (kJ/mol):
\begin{itemize}
  \item 35.54, 32.11 (25°C, bp, Dreisbach 1961)
  \item 35.74, 31.80 (25°C, bp, Riddick et al. 1986)
\end{itemize}
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: 1.0
Water Solubility (g/m$^3$ or mg/L at 25°C):
\begin{itemize}
  \item miscible (Dean 1985; Howard 1990; Yaws et al. 1990)
  \item miscible (Riddick et al. 1986)
  \item miscible (Stephenson 1993b)
\end{itemize}
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\begin{itemize}
  \item 13850 (Hoy 1970; Abraham 1984)
  \item 12230 (calculated by formula, Dreisbach 1961)
\end{itemize}
\begin{align*}
\log (P/\text{mmHg}) &= 7.213 – 1308.4/(224.2 + t/°C); \text{temp range 4–114°C (Antoine eq. for liquid state, Dreisbach 1955)} \\
9600 &= (20°C, Verschueren 1983) \\
12230 &= \text{quoted lit., Riddick et al. 1986; quoted, Howard 1990) and Antoine eq. for liquid state, Dreisbach 1955)} \\
12520 &= \text{extrapolated-Antoine eq., Stephenson & Malanowski 1987)} \\
12520 &= \text{extrapolated-Antoine eq., Stephenson & Malanowski 1987)}
\end{align*}
\begin{align*}
\log (P/\text{kPa}) &= 6.2635 – 1258.745/(-54.49 + T/K); \text{temp range 313–350 K (Antoine eq., Stephenson & Malanowski 1987)} \\
\log (P/\text{mmHg}) &= 25.0711 – 2.5701 \times 10^3/(T/K) – 5.8985 \log (T/K) + 7.9399 \times 10^{-10} (T/K) + 1.192 \times 10^{-6} (T/K)^2; \text{temp range 124–532 K (vapor pressure eq., Yaws 1994)}
\end{align*}
Henry’s Law Constant (Pa m$^3$/mol at 25°C):
\begin{itemize}
  \item 1.526 (partial pressure, Butler & Ramchandani 1935)
  \item 1.528 (exptl., Hine & Mookerjee 1975)
\end{itemize}
Nitrogen and Sulfur Compounds

1.676, 1.68 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.880 (calculated-molecular structure, Russell et al. 1992)
1.785 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 0.68 (shake flask, Collander 1951)
- 0.88 (shake flask-titration, Sandell 1962)
- 0.81 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1987)
- 0.74 (shake flask-titration, Korenman et al. 1973)
- 0.90, 0.92; 0.81 (calculated-$f$ const.; calculated-$\pi$ const., Rekker 1977)
- 0.80 (inter-lab. shake flask average, Eadsforth & Moser 1983)
- 0.97 (shake flask-GC, Takayama et al. 1985)
- 0.86 (recommended, Sangster 1989)
- 0.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 3.61 (calculated-$S_{oct}$ and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
- 0.505 (calculated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log $K_{OC}$:
- 1.903 (soil, calculated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1990)
- 1.176, 2.021, 2.029 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.880 (soil, quoted exptl., Meylan et al. 1992)
- 1.780 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:
Volatilization: using Henry’s law constant, $t_1/2 = 1.95$ d was predicted for evaporation from a model river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).
Photolysis:
Oxidation: estimated vapor phase photooxidation $t_1/2 = 0.479$ d in air, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of $5 \times 10^5$ radicals/cm$^3$ (USEPA 1986; quoted, Howard 1990).

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: estimated vapor phase $t_1/2 = 0.479$ d, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of $5 \times 10^5$ radicals/cm$^3$ (USEPA 1986; quoted, Howard 1990).
16.1.2.7 Ethanolamine

Common Name: Ethanolamine
Synonym: β-aminoethyl alcohol, ethylolamine, 2-hydroxyethylamine, β-hydroxyethylamine, monoethanolamine, MEA
Chemical Name: ethanolamine, 2-aminoethanol
CAS Registry No: 141-43-5
Molecular Formula: C₂H₇NO, HOCH₂CH₂NH₂
Molecular Weight: 61.098
Melting Point (°C): 10.5 (Lide 2003)
Boiling Point (°C): 171 (Lide 2003)
Density (g/cm³ at 20°C): 1.0180 (Weast 1982–83)
Molar Volume (cm³/mol): 60.4 (Stephenson & Malanowski 1987)
Enthalpy of Vaporization, ΔHV (kJ/mol): 92.09, 49.831 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol): 20.50 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus J/mol K: Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Dean 1985)
miscible (Riddick et al. 1986; quoted, Howard 1990)

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):
893* (65.4°C, Ramsay-Young method, measured range 65.4–170.9°C, Matthews et al. 1950)
log (P/mmHg) = 44.008 – 4089/(T/K) – 11.446 ± log (T/K); temp range 65.4–170.9°C (Kirchhoff eq., ebulliometry, Matthews et al. 1950)
8707* (106.1°C, ebulliometry, measured range 106.1–170.37°C, McDonald et al. 1959)
log (P/mmHg) = 7.7380 – 1772.11/(185.56 + t/°C); temp range 106–170°C, or pressure range 65.31–760 mmHg (ebulliometry, McDonald et al. 1959)
53.32 (20°C, Verschuuren 1983)
41.64, 46.67 (extrapolated values-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 6.54175 – 1554.149/(171.175 + t°C); temp range 65.5–170.9°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
log (P/kPa) = 6.86239 – 1725.168/(185.56 + t°C); temp range 106.1–170.37°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
42.51 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.4568 – 1577.67/(172.37 + t°C); temp range 65–171°C (Antoine eq., Dean 1985, 1992)
48.0 (Riddick et al. 1986)
log (P/kPa) = 6.86290 – 1732.11/(186.215 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
47.34 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.8629 – 1732.11/(86.6 + T/K); temp range 310–444 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
34.66 (from Dow Chemical's Handbook, Howard 1990)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 72.9125 - 5.8595 \times 10^3 \left( \frac{T}{\text{K}} \right) - 7.1511 \times 10^{-10} \left( \frac{T}{\text{K}} \right)^2 + 5.9841 \times 10^{-6} \left( \frac{T}{\text{K}} \right)^3 \]

temp range 284–638 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):

0.0041 (calculated-bond method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):

-1.31 (shake flask, Collander 1951)
-1.29; -1.35 (calculated-f const., calculated-\( \pi \) const., Rekker 1977)
-1.31 (recommended, Sangster 1993)
-1.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):

Bioconcentration Factor, log \( \text{BCF} \):

< 0.0 (estimated-\( K_{\text{OW}} \), Lyman et al. 1982; quoted, Howard 1990)

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

0.699 (soil, estimated-\( K_{\text{OW}} \), Lyman et al. 1982; quoted, Howard 1990)

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

Volutilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation \( t_{1/2} = 11 \text{ h in air} \), based on an estimated rate constant \( k \approx 3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \)

for the vapor phase reaction with photochemically produced hydroxyl radical of \( 5 \times 10^5 \text{ radicals/cm}^3 \) in air


Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: half-life of 11 h, based on an estimated rate constant of \( 3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor phase reaction with photochemically produced hydroxyl radical of \( 5 \times 10^5 \text{ radicals/cm}^3 \) in air (Atkinson 1987; quoted, Howard 1990).
TABLE 16.1.2.7.1
Reported vapor pressures of ethanolamine at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1)
\]

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

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

Matthews et al. 1950

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<th>t/°C</th>
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<td>75.4</td>
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<td>96.4</td>
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<td>ΔH_v/(kJ mol(^{-1})) = 46.07 at bp</td>
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<td>B</td>
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<td>C</td>
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McDonald et al. 1959

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**FIGURE 16.1.2.7.1** Logarithm of vapor pressure versus reciprocal temperature for ethanolamine.
16.1.2.8 Diethanolamine

Common Name: Diethanolamine
Synonym: 2,2'-amino-dietanol, 3-aza-1,5-pentanediol, diethylolamine, bis(hydroxyethyl)amine, 2,2'-dihydroxydiethylamine, β,β'-dihydroxydiethylamine, 2,2'-iminobisethanol, 2,2'-iminodiethanol
Chemical Name: diethanolamine
CAS Registry No: 111-42-2
Molecular Formula: C₄H₁₁NO₂, HOCH₂CH₂NHCH₂CH₂OH
Molecular Weight: 105.136

Melting Point (°C):
28.0 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
268.8 (Lide 2003)

Density (g/cm³ at 20°C):
1.0966 (Weast 1982–83)
1.0936 (25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
96.5 (30°C, Stephenson & Malanowski 1987)
126.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:
8.88, 8.97 (Perrin 1972)
8.88 (pKᵢ⁻, Dean 1985; Riddick et al. 1986)

Enthalpy of Vaporization, ΔHV (kJ/mol):
70.3, 65.229 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔHfus (kJ/mol):
25.104 (Riddick et al. 1986)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.934 (mp at 28°C)

Water Solubility (g/m³ or mg/L at 25°C):
954000 (Verschueren 1983)
964000 (Dean 1985)
954000 (20°C, Riddick et al. 1986)
miscible (from Dow Chemical’s Handbook, Howard 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
< 1.333 (20°C, Verschueren 1983)
0.040 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 8.1388 – 2327.9/(174.4 + t°C); temp range 194–241°C (Antoine eq., Dean 1985, 1992)
0.030 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 7.26458 – 2328.56/(174.399 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 7.2644 – 2326.23/(–98.907 + T/K); temp range: 423–542 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
0.0373 (quoted from Dow Chemical’s Handbook, Howard 1990)
log (P/mmHg) =122.0877 –8.8422 × 10⁻³/(T/K) –40.422·log (T/K) + 1.4062 × 10⁻²·(T/K) + 1.1986 × 10⁻¹²·(T/K)²; temp range 301–542 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
5.42 × 10⁻⁹ (Hine & Mookerjee 1975)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- $-1.43$ (shake flask, Collander 1951)
- $-1.51$ (calculated-fragment const., Rekker & De Kort 1979)
- $-1.43$ (recommended, Sangster 1993)
- $-1.43$ (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- $< 0.0$ (estimated-$K_{OW}$, Howard 1990)

Sorption Partition Coefficient, log $K_{OC}$:
- $0.602$ (soil, estimated-$K_{OW}$, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation: photooxidation $t_\frac{1}{2} = 0.72–7.2$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991).
- Biodegradation: aqueous aerobic $t_\frac{1}{2} = 14.4–168$ h, based on measured half-life in surface water grab sample experiment (Boethling & Alexander 1979; quoted, Howard et al. 1991) and aqueous aerobic screening test data (Gerike & Fischer 1979; Bridie et al. 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_\frac{1}{2} = 57.6–672$ 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: photooxidation $t_\frac{1}{2} = 0.72–7.2$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991); atmospheric transformation lifetime by reaction with water was estimated to be $< 1$ d (Kelly et al. 1994).
- Surface water: $t_\frac{1}{2} = 14.4–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Groundwater: $t_\frac{1}{2} = 28.8–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment:
- Soil: $t_\frac{1}{2} = 14.4–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Biota:
16.1.2.9 Triethanolamine

Common Name: Triethanolamine
Synonym: 2,2',2''-nitrilotriethanol, 2,2',2''-nitrilotrisethanol, triethylolamine, trihydroxytriethylamine, trolamine, tris(hydroxyethyl)-amine, TEA
Chemical Name: triethanolamine
CAS Registry No: 102-71-6
Molecular Formula: C_6H_{15}NO_3, (HOCH_2CH_2)_3N
Molecular Weight: 149.188
Melting Point (°C):
   20.5 (Lide 2003)
Boiling Point (°C):
   335.4 (Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
   1.1242 (Weast 1982–83; Dean 1985)
   1.1196 (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
   133.3 (Stephenson & Malanowski 1987)
   182.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
   7.92 (Perrin 1972; quoted, Howard 1990)
   7.76 (pK_BH^+, Dean 1985; Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
   67.475 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   27.20 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Water Solubility (g/m³ or mg/L at 25°C):
   miscible (Dean 1985; Howard 1990)
   miscible (Riddick et al. 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   < 1.33 (20°C, Verschueren 1983)
   0.0131 (extrapolated-Antoine eq., Boublik et al. 1984
   log (P/kPa) = 9.19319 – 4543.817/(297.839 + t/°C), temp range: 252.7–305.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   0.0100 (extrapolated-Antoine eq., Dean 1985, 1992)
   log (P/mmHg) = 10.0675 – 4542.78/(297.76 + t/°C), temp range: 252–305°C (Antoine eq., Dean 1985, 1992)
   < 1.30 (20°C, Riddick et al. 1986)
   log (P/kPa) = 7.67989 – 2962.73/(186.75 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
   4.79 × 10⁻⁴ (quoted from Dow Chemical’s Handbook, Howard 1990)
   log (P/mmHg) = 135.3206 – 1.0312 × 10⁹/(T/K) – 44.637·log (T/K) + 1.4368 × 10⁻²·(T/K) – 1.7552 × 10⁻¹³·(T/K)²;
   temp range 294–787 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   3.42 × 10⁻¹⁴ (Hine & Mookerjee 1975)
Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
-1.32, -1.75 (calculated, Verschueren 1983)
-1.59 (Howard 1990)
-1.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:

Bioconcentration Factor, log BCF:
< 0.0 (estimated-$K_{\text{OW}}$, Howard 1990)

Sorption Partition Coefficient, log $K_{\text{OC}}$:
0.477 (soil, estimated-$K_{\text{OW}}$, Howard 1990)

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

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: photooxidation $t_\text{1/2} = 4.0$ h in air, based on an estimated rate constant $k \sim 10.4 \times 10^{-11}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5$ radicals/cm$^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).

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

Half-Lives in the Environment:
Air: $t_\text{1/2} = 4.0$ h, based on an estimated rate constant $k \sim 10.4 \times 10^{-11}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5$ radicals/cm$^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).
16.1.3 AROMATIC AMINES

16.1.3.1 Aniline

Common Name: Aniline
Synonym: phenylamine, aminobenzene, benzeneamine, benzenamine
Chemical Name: aniline
CAS Registry No: 62-53-3
Molecular Formula: C₆H₅NH₂
Molecular Weight: 93.127
Melting Point (°C): –6.02 (Lide 2003)
Boiling Point (°C): 184.1 (Lide 2003)
Density (g/cm³ at 20°C):
- 1.02173, 1.01750 (20°C, 25°C, Dreisbach 1955)
- 1.02173 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
- 91.2 (20°C, calculated-density)
- 110.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
- 4.596 (Perrin 1972; Howard 1989)
- 4.600 (McLeese et al. 1979; Riddick et al. 1986; Sangster 1989)
- 4.630 (Weast 1982–83)
- 4.58, 3.96 (quoted, HPLC, Miyake et al. 1987)
Enthalpy of Vaporization, ΔHV (kJ/mol):
- 54.28, 43.17 (25°C, bp, Dreisbach 1955)
- 55.843, 44.53 (25°C, bp, Riddick et al. 1986)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
- 36650 (Hill & Macy 1924)
- 36070 (Seidell 1941)
- 38670 (shake flask-residue volume method, Booth & Everson 1948)
- 36220 (shake flask-interferometry, Donahue & Bartell 1952)
- 34100 (Stephen & Stephen 1963)
- 36600 (Kenaga 1980)
- 34000 (Verschueren 1983)
- 56900 (calculated-activity coeff. γ by UNIFAC, Fu & Luthy 1985, 1986)
- 33800 (selected, Riddick et al. 1986)
- 34200 (selected, Yaws et al. 1990)
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 (43.7°C, static method, measured range 43.7–183.9°C, Kahlbaum 1898)
- 85.71* (extrapolated-regression of tabulated data, temp range 34.8–184.4°C Stull 1947)
log (P/mmHg) = 7.57170 – 1941.7/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
10351* (112.92°C, ebulliometry, measured range 112.92–183.93°C, Dreisbach & Shrader 1949)
89.52 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986)
log (P/mmHg) = 7.24179 – 1674.3/(200.0 + t°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

6806* (102.59°C, ebulliometry, measured range 102.59–185.15°C, McDonald et al. 1959)

log (P/mmHg) = 7.25375 – 1684.35/(201.175 + t°C), temp range 103–185°C (Antoine eq., ebulliometry, McDonald et al. 1959)

133.3* (31.55°C, calculated-thermodynamic properties, temp range 31.55–184.40°C, Hatton et al. 1962)

log (P/mmHg) = –0.2185 × 11307.6/(T/K) + 8.221995; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

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

log (P/mmHg) = 7.32010 – 1731.515/(206.049 + t°C); temp range 102–185°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.32010 – 1731.515/(206.049 + t°C); temp range 102–185°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.43196 – 1722.154/(205.002 + t°C); temp range 102.6–185.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.69066 – 1941.7/(230.0 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.69066 – 1941.7/(230.0 + t°C) (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.69066 – 1941.7/(230.0 + t°C) (extrapolated-Antoine eq., Boublik et al. 1984)

Henry’s Law Constant (Pa·m3/mol at 25°C):

13778 (Hakuta et al. 1977)

12.16 (measured, Yoshida et al. 1983)

Octanol/Water Partition Coefficient, log K\text{OW}:

0.90 (shake flask-UV, Fujita et al. 1964)

0.90 (shake flask, Iwasa et al. 1965)

0.90 (shake flask-UV, Hansch et al. 1968)

0.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1983, Hansch & Leo 1985)

0.89 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

0.90 (HPLC-K’ correlation, Carlson et al. 1975)

0.85 (shake flask, Lu & Metcalf 1975)

0.90 (HPLC-RT correlation, Mirrlees et al. 1976)

0.93 ± 0.05 (shake flask at pH 7, Unger et al. 1978)

0.90, 0.98, 0.85 (shake flask, Hansch & Leo 1979)

0.91 (HPLC-K’ correlation, Könenmann et al. 1979)

0.90 (shake flask-UV, Briggs 1981)
Nitrogen and Sulfur Compounds

1.03  (RP-HPLC-k' correlation, D’Amboise & Hanai 1982)
0.90  (HPLC-k' correlation, Hammers et al. 1982)
0.90  (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
1.09  (inter-laboratory studies, HPLC-RT correlation, average, Eadsforth & Moser 1983; Brooke et al. 1990)
1.34, 1.27, 1.08 (HPLC-RT correlation, Harnish et al. 1983)
1.08  (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
0.79, 0.96 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.89  (shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.99  (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
0.81, 1.08 (HPLC-k' correlation, Eadsforth 1986)
0.91  (RP-HPLC-RT correlation, Eadsforth 1986)
0.98  (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
0.93  (HPLC method average, Ge et al. 1987)
0.78  (HPLC-k' correlation, Miyake et al. 1987)
1.18  (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.94 ± 0.006 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
0.90  (recommended, Sangster 1989, 1993)
0.942 ± 0.010; 0.940 ± 0.006 (shake flask/stir-flask method by BRE; RITOX, inter-laboratory studies, Brooke et al. 1990)
0.90  (shake flask-GC, Alcorn et al. 1993)
1.21, 0.89, 0.87, 1.09 (HPLC-k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
0.92  (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)
0.88  (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

0.78  (fish, Lu & Metcalf 1975)
0.30  (calculated-S, Kenaga 1980)
< 1.0 (fish, Freitag et al. 1982)
< 1.0, 0.602, 3.01 (golden orfe, algae, activated sludge, Freitag et al. 1982)
0.602 (alga Chlorella fusca, wet wt. basis, Geyer et al. 1984)
0.845 (alga Chlorella fusca, calculated-$K_{OW}$, Geyer et al. 1984)
< 1.0, < 1.0, 2.70 (golden ide, algae, activated sludge, Freitag et al. 1985)
2.77  (Daphnia magna, based on elimination phase, Dauble et al. 1986)
1.87  (Daphnia magna, based on $^{14}$C and exposure water, Dauble et al. 1986)
0.70  (fish, correlated-$K_{OW}$, Isnard & Lambert 1988)
0.78 (quoted, Isnard & Lambert 1988, 1989)
0.41 (zebrafish, Kalsch et al. 1991)
0.41 (zebrafish, Zok et al. 1991)
0.41; 1.04, -0.87, 0.03 (quoted exptl.; calculated values-$K_{OW}$, Bintein et al. 1993)

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

3.11; 2.11 (H-montmorillonite at pH 8.35; pH 6.80, Bailey et al. 1968)
1.86  (soil average, Moreale & Van Bladel 1976)
1.41  (average of seven agricultural soils, Briggs 1981)
3.59  (colloidal organic carbon/ground water, Means et al.1982)
2.11; 2.61 (soil; more acidic soil, Pillai et al. 1982)
2.49; 2.11 (nonsterile Hagerstown soil; sterile Hagerstown soil, Pillai et al. 1982)
2.96; 2.61 (nonsterile Palouse soil; sterile Palouse soil, Pillai et al. 1982)
1.17  (soil, quoted as log $K_{OM}$, Sabljic 1987)
2.12, 2.05, 2.06 (calculated values: Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
0.596 (calculated-$K_{OM}$, Kollig 1993)
1.08, 1.25, 0.98 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)
1.41 (soil, calculated-MCI 1, Szabljic et al. 1995)
2.07; 1.65 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.70, 1.64, 2.08, 2.04, 2.29 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.38, 1.50, 1.27, 2.13 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
1.0–1.54 (5 soils, pH 2.8–7.2, batch equilibrium-sorption isotherm, Li et al. 2000)

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

Volatilization: estimated $t_{1/2} = 12$ d from a measured Henry’s law constant of $1.2 \times 10^{-4}$ atm m$^3$ mol$^{-1}$ (Yoshida et al. 1983; quoted, Howard 1989) for a model river of 1-m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989); volatilization $t_{1/2}(calc) = 55$ d (Toräng et al. 2002).

Photolysis: first-order rate constants for photosensitized reactions in water with various humic substances as sensitizers: $k = 0.17$ h$^{-1}$ with aquatic humus from Aucilla River, $k = 0.12$ h$^{-1}$ with Aldrich humic acid, $k = 0.091$ h$^{-1}$ with Fluka humin acid and $k = 0.11$ h$^{-1}$ with Contech fulvic acid in sunlight, corresponding to half-lives of 4 to 8 h (Zepp et al. 1981); photolysis $t_{1/2} = > 50$ yr at 15°C and a pH 5–9 (Toräng et al. 2002).

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:

$k = 1 \times 10^{4}$ M$^{-1}$ s$^{-1}$ for oxidation by RO$_2$ radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
$k < 2 \times 10^{6}$ M$^{-1}$ s$^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)
$k_{OH} = 1.20 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(av.) = 1.17 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (flash photolysis -RF, Rinke & Zetzsch 1984; Witte et al. 1986)
$k_{OH} = 1.10 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range: 239–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)
$k_{OH}(calc) = 1.54 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson et al. 1985)
$k_{OH}(obs) = 6.0 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH}(calc.) = 1.16 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1985)
$k_{OH}(calc) = 1.36 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 1.17 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (SAR structure-activity relationship, Atkinson 1987)
$k_{OH}^{*}(exptl) = 1.18 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K, measured range: 265–455 K; and $k_{OH} = 1.12 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)
$k_{OH}^{*} = 1.11 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
$k_{OH}(calc) = 1.385 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: completely degraded by a soil inoculum in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983; Howard 1989); completely degraded in 20 d by bacteria in river mud (Calamari et al. 1980; quoted, Howard 1989); $k = 0.23$ d$^{-1}$ and corresponding to a $t_{1/2} = 3$ d in samples of White Lake water at 29°C (Subba-Rao et al. 1982);
average rate of biodegradation $k = 19.0$ mg COD g$^{-1}$ h$^{-1}$ for 94.5% removal (Scow 1982);
biodegradation $t_{1/2} = 4.5$ d in unpolluted and $t_{1/2} < 0.5$ d in polluted pond water as model environments (Lyons et al. 1984);
0.46 mM aniline solution degraded by strain Ani1 within 14 d in water (Schnell et al. 1989); average exptl. k = 0.044 h$^{-1}$ compared to the group-contribution method predicted rate constants of 0.050 h$^{-1}$ (nonlinear) and 0.018 h$^{-1}$ (Tabak & Govind 1993);

first-order $k = 1.0$ d$^{-1}$ for batch expt. with Elbe water at 20°C (Börnick et al. 2001);
field first-order degradation $k \approx 1.8$ d$^{-1}$ for 2 different dates with water temperatures of 21.9 and 14.7°C, respectively, in Rhine river and rate constant obtained in laboratory shake flask batch tests with Rhine water averaged 1.5 d$^{-1}$ at 15°C and 2.0 d$^{-1}$ at 20°C (Toräng et al. 2002).
Biotransformation: mean bacteria transformation rate constant for all three sites of \((1.1 \pm 0.8) \times 10^{-11}\) L·organism⁻¹·h⁻¹ (Paris & Wolfe 1987; quoted, Steen 1991).

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:

\[
k_1 = 0.052 \pm 0.0067 \, \text{h}^{-1}; \quad k_2 = 7.200 \pm 1.3000 \, \text{h}^{-1} \quad (\text{Kalsch et al. 1991})
\]

\[
k_1 = 11.10 \pm 3.2000 \, \text{h}^{-1} \quad (\text{zebrafish, Zok et al. 1991})
\]

Half-Lives in the Environment:

Air: atmospheric lifetimes of 2.3 h in clean troposphere and 1.2 h in moderately polluted atmosphere, based on gas-phase reaction with hydroxyl radical at room temp.; atmospheric lifetimes of 15.0 d in clean troposphere and 5.0 d in moderately polluted atmosphere, based on gas-phase reaction with \(O_3\) at room temp. (Atkinson et al. 1987)

\[
t_{1/2} \sim 3.3 \, \text{h}, \quad \text{based on reaction with photochemically produced hydroxyl radical (Howard 1989);}
\]

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated \(t_{1/2} = 2.3\) d in Rhine river in case of a first order reduction process (Zoeteman et al. 1980; quoted, Howard 1989);

Estimated \(t_{1/2} = 0.3–3.0\) d in river waters (Zoeteman et al. 1980); \(t_{1/2} = 4\) to 8 h in May sunlight with both commercial humic acids and aquatic humus as photosensitizers near-surface water and \(t_{1/2} \sim 1\) wk in distilled water (Zepp et al. 1981);

\(t_{1/2} = 6\) d in eutrophic pond and \(t_{1/2} = 21\) d in an oligotrophic lake (Subba-Rao et al. 1982; quoted, Howard 1989); biodegradation \(t_{1/2} = 4.5\) d in unpolluted and \(t_{1/2} < 0.5\) d in polluted pond water as model environments (Lyons et al. 1984);

\(t_{1/2} = 4–33\) d at 15°C (Ingerslev & Nyholm 2000);

\(t_{1/2} \sim 9\) h in the Rhine river at 15 and 22°C (Toräng et al. 2002).

Ground water: estimated \(t_{1/2} \sim 30−300\) d (Zoeteman et al. 1980).

Sediment:

Soil:

Biota:

---

### TABLE 16.1.3.1.1

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

<table>
<thead>
<tr>
<th>Summary of literature data</th>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>McDonald et al. 1959</th>
<th>Hatton et al. 1962</th>
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<td>(P/Pa)</td>
<td>(t/°C)</td>
<td>(P/Pa)</td>
<td>(t/°C)</td>
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<td>101325</td>
<td>bp/°C</td>
<td>183.93</td>
<td>184.24</td>
</tr>
</tbody>
</table>

\(P/mmHg\) & \(A\) & \(7.25375\) & \(B\) & \(1684.35\) & \(C\) & \(201.175\) |
FIGURE 16.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for aniline.
16.1.3.2 2-Chloroaniline

Nitrogen and Sulfur Compounds

NH₂
Cl

Common Name: 2-Chloroaniline
Synonym: 1-amino-2-chlorobenzene, o-aminochlorobenzene, o-chloroaniline, 2-chlorophenylamine
Chemical Name: 1-amin o-2-chlorobenzene, o-chloroaniline, 2-chloroaniline
CAS Registry No: 95-51-2
Molecular Formula: C₆H₄NH₂Cl
Molecular Weight: 127.572

Melting Point (°C):
-1.94 (β-2-chloroaniline, Dreisbach 1955; Weast 1872–83, Riddick et al. 1986)
-14.0 (α-2-chloroaniline, Weast 1982–83; Verschuuren 1983; Howard 1989)
-1.9 (Lide 2003)

Boiling Point (°C):
208.8 (Kahlbaum 1898; Stull 1947; Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
1.21266, 1.20787 (20°C, 25°C, Dreisbach 1955)
1.21251, 1.20775 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
105.2 (20°C, Stephenson & Malanowski 1987)
131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
2.661 (Perrin 1972; quoted, Howard 1989)
2.650 (Weast 1982–83)
2.640 ( protonated cation + 1, Dean 1985)
2.640 (Riddick et al. 1986)

Enthalpy of Vaporization, ∆HV (kJ/mol):
57.5 ± 5 (25°C, Piacente et al. 1985)
56.756, 44.35 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ∆Hfus (kJ/mol):
11.88 (Riddick et al. 1986)

Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
8760 (Dreisbach 1955)
3765 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
3763 (calculated-Kow, Müller & Klein 1992)
4740 (calculated-group contribution method, Kühne et al. 1995)

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):
40.31* (extrapolated-regression of tabulated data, measured range 64.4–208.8°C, Kahlbaum 1898)
37.77* (extrapolated-regression of tabulated data, temp range 46.3–208.8°C, Stull 1947)
log (P/mmHg) = 7.63311 – 2085.5/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
7605* (124.48°C, ebulliometry, measured range 124.48–208.84°C, Dreisbach & Shrader 1949)
33.77 (calculated by formula, Dreisbach 1955; selected, Riddick et al. 1986)
log (P/mmHg) = 7.19240 – 1762.74/(200.0 + t°C); temp range 110–330°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [−0.2185 × 12441.0/(T/K)] + 8.56946; temp range 46.3–208.8°C (Antoine eq., Weast 1972–73)
33.88 (calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = 7.56265 - 1998.6/(220.0 + t/\degree\text{C}), \text{ temp range 20–108}\degree\text{C} \text{ (Antoine eq., Dean 1985, 1992)}
\]
\[
\log (P/\text{mmHg}) = 7.19240 - 1762.74/(200.0 + t/\degree\text{C}), \text{ temp range: 108–300}\degree\text{C} \text{ (Antoine eq., Dean 1985, 1992)}
\]
\[
\log (P/\text{mmHg}) = (8.63 \pm 0.16) - (3006 \pm 56)/(T/\text{K}); \text{ temp range: 287–336 K} \text{ (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)}
\]
\[
\log (P/\text{mmHg}) = 6.75801 - 2085.50/(230.0 + t/\degree\text{C}); \text{ temp range not specified} \text{ (Antoine eq., Riddick et al. 1986)}
\]
\[
\log (P/\text{mmHg}) = 90.6491 - 6.041 \times 10^3/(T/\text{K}) - 31.118\cdot\log (T/\text{K}) + 1.1564 \times 10^{-2}\cdot(T/\text{K}) + 4.8388 \times 10^{-13}\cdot(T/\text{K})^2; \text{ temp range 271–722 K} \text{ (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.760 (calculated-P/C, Howard 1989)
- 0.425 (calculated-P/C, Meylan & Howard 1991)
- 0.143 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
- 1.81 (shake flask, Fujita et al. 1964)
- 1.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
- 1.92 (exptl., Leo et al. 1971; McCall 1975; Rekker 1977)
- 1.92 (HPLC-\(k’\) correlation, Carlson et al. 1975)
- 1.63 (calculated-\(\pi\) const., Norrington et al. 1975)
- 1.61, 1.73 (calculated-\(\pi\) const., calculated-\(\pi\) const., Rekker 1977)
- 1.90, 1.92 (shake flask, Hansch & Leo 1979)
- 1.74 (HPLC-\(k’\) correlation, Könemann et al. 1979)
- 1.74 (calculated-\(\pi\) const., Rekker & De Kort 1979)
- 1.91 \pm 0.01 (HPLC-\(k’\), Hammers et al. 1982)
- 1.99 (HPLC-\(k’\) correlated, Hammers et al. 1982)
- 1.926 \pm 0.021 (slow-stirring-GC, De Brujin et al. 1989)
- 1.88 (recommended, Sangster 1993)
- 1.93 \pm 0.14, 1.55 \pm 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
- 1.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\):

Bioconcentration Factor, log \(BCF\):
- < 2.0 (Kawasaki 1980)
- 1.30 (estimated, Canton et al. 1985)
- 1.18 (zebrafish, Zok et al. 1991)
- 0.301–0.57 (carp, Tsuda et al. 1993)
- 1.18; 1.56, 0.73, 0.94 (quoted; calculated values-\(K_{\text{OW}}\), Bintein et al. 1993)

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

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
- Volatilization: using Henry’s law constant, \(t_{1/2} \sim 5.6\ \text{d} \) was estimated for a model river of 1-m deep (Lyman et al. 1982; quoted, Howard 1989); estimated \(t_{1/2} = 64\ \text{d} \) from a representative environmental pond (stagnant) (USEPA 1987; quoted, Howard 1989).
- Photolysis: Oxidation: rate constant of \(5.1 \times 10^{-12}\ \text{cm}^3\text{molecule}^{-1}\text{s}^{-1}\) for the reaction with hydroxyl radical in a typical ambient atmosphere at 25°C with \(t_{1/2} \sim 2\ \text{d} \) (GEMS 1987; quoted, Howard 1989).
- Hydrolysis: Biodegradation: average biodegradation rate of 25 mg COD g⁻¹ h⁻¹ for 95.6% removal (Scow 1982).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

\[ k_1 = 7.10 \, \text{h}^{-1} \, (\text{zebrafish}, \text{Zok et al. 1991}) \]

\[ k_2 = 0.19 \, \text{h}^{-1} \, (\text{carp}, \text{Tsuda et al. 1993}) \]

Half-Lives in the Environment:
Air: estimated atmospheric $t_{1/2} = 2 \, \text{d}$, based on the reaction with sunlight-produced hydroxyl radical (GEMS 1987; quoted, Howard 1989).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{1/2} = 3.6 \, \text{h}$ in carp with excretion rate constant $k = 0.19 \, \text{h}^{-1}$ (Tsuda et al. 1993).

### TABLE 16.1.3.2.1
Reported vapor pressures of 2-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Kahlbaum 1898 static method</th>
<th>Stull 1947 summary of literature data</th>
<th>Piacente et al. 1985 torsion-weighing effusion</th>
<th>Piacente et al. 1985 torsion-weighing effusion</th>
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<tbody>
<tr>
<td>$P/\text{Pa}$</td>
<td>$P/\text{Pa}$</td>
<td>$P/\text{Pa}$</td>
<td>run 62 average</td>
<td>$P/\text{Pa}$ average</td>
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<tr>
<td>64.4</td>
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<td>14</td>
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<td>72.3</td>
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<td>84.8</td>
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<td>343</td>
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<td>199.4</td>
<td>79993</td>
<td></td>
<td>56</td>
<td>354</td>
</tr>
<tr>
<td>208.8</td>
<td>101325</td>
<td></td>
<td>57</td>
<td>398</td>
</tr>
</tbody>
</table>

**Dreisbach & Shrader 1949**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$P/\text{Pa}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>124.48</td>
<td>7605</td>
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<tr>
<td>131.54</td>
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<td>145.3</td>
<td>16500</td>
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<td>154.55</td>
<td>42066</td>
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<td>192.71</td>
<td>67661</td>
</tr>
<tr>
<td>208.84</td>
<td>101325</td>
</tr>
</tbody>
</table>

Overall vapor pressure eq.:

$\Delta H_v/(\text{kJ mol}^{-1}) = 57.5 \pm 5$

at 25°C

\[ A = 8.63 \pm 0.16 \]

\[ B = 3006 \pm 56 \]
FIGURE 16.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-chloroaniline.
16.1.3.3  3-Chloroaniline

Common Name: 3-Chloroaniline
Synonym: 1-amino-3-chlorobenzene, m-chloroaniline, 3-chlorophenylamine
Chemical Name: 1-amino-3-chlorobenzene, m-chloroaniline, 3-chloroaniline
CAS Registry No: 108-42-9
Molecular Formula: C₆H₄NH₂Cl
Molecular Weight: 127.572

Melting Point (°C):
-10.28  (Lide 2003)

Boiling Point (°C):
230.5  (Lide 2003)

Density (g/cm³ at 20°C):
1.21606  (20°C, Weast 1982–83)
1.2150  (22°C, Dean 1985; Budavari 1989)

Molar Volume (cm³/mol):
105.0  (22°C, calculated-density, Stephenson & Malanowski 1987)
131.1  (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
3.52  (Perrin 1972)
3.50  (McLeese et al. 1979)
3.46  (Weast 1982–83)
3.52  (protonated cation + 1, Dean 1985)

Enthalpy of Vaporization, Δ Hv (kJ/mol):
61.04, 46.016  (25°C, bp, Dreisbach 1955)
60.9 ± 5  (25°C, Piacente et al. 1985)

Enthalpy of Fusion, Δ Hfus (kJ/mol):
10.25  (Dreisbach 1955)

Entropy of Fusion, Δ Sfus (J/mol K):

Fugacity Ratio at 25°C (assuming Δ Sfus = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
5442  (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
5447  (calculated-K Ow, Müller & Klein 1992)
4740  (calculated-group contribution method, Kühne et al. 1995)

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):
13.14*  (extrapolated-regression of tabulated data, measured range 81.7–228.5°C, Kahlbaum 1898)
11.94*  (extrapolated-regression of tabulated data, temp range 63.5–228.5°C, Stull 1947)
11.17  (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 7.23603 – 1857.75/(196.64 + t°C); temp range 125–350°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/mmHg) = [–0.2185 × 133854.6/(T/K)] + 8.761546; temp range 63.5–228.5°C (Antoine eq., Weast 1972–73)

11.06  (calculated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.59939 – 2073.75/(215.0 + t°C), temp range 15–125°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.23603 – 1857.75/(196.64 + t°C), temp range 125–310°C (Antoine eq., Dean 1985, 1992)
15.60*  (torsion-weighing effusion, Piacente et al. 1985)
log (P/kPa) = (8.86 ± 0.10) – (3180 ± 40)/(T/K); temp range ~290–345 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
9.530 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.36093 – 1857.75/(–76.51 + T/K); temp range 398–573 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 65.6033 – 5.3779 × 10^3/(T/K) – 20.518·log (T/K) + 6.7861 × 10^-3·(T/K) + 2.1167 × 10^-13·(T/K)^2; temp range 263–751 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
0.223 (calculated-P/C)
0.102 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.88 (shake flask-UV, Fujita et al. 1964)
1.88 (Ichikawa et al. 1969)
1.88 (Leo et al. 1971; Hansch & Leo 1979)
1.90 (exptl., Leo et al. 1971; Rekker 1977)
1.98 (calculated-π const., Norrington et al. 1975)
1.73, 1.75; 1.61 (calculated-f const., calculated-π const., Rekker 1977)
1.90, 1.88 (shake flask, Hansch & Leo 1979)
1.57 (HPLC-k’ correlation, Könenmann et al. 1979)
1.89 ± 0.01 (HPLC-k’ correlation, Hammers et al. 1982)
2.00 (HPLC-k’ correlation, Hammers et al. 1982)
1.910 ± 0.013 (slow-stirring-GC, De Bruijn et al. 1989)
1.88 (recommended, Sangster 1993)
1.91 ± 0.14, 1.52 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k’ correlation, Cichna et al. 1995)
1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.06 (zebrafish, Zok et al. 1991)
–0.097 to 0.342 (average for carp, Tsuda et al. 1993)
1.06; 1.55, 0.70, 0.92 (quoted; calculated values, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:
Photolysis: direct aqueous photolysis rate constant k = 0.393 ± 0.006 min^{-1} with a calculated t_{1/2} = 1.76 min (Stegeman et al. 1993).

Oxidation:

Hydrolysis: direct photohydrolysis rate constant k = 0.393 ± 0.006 min^{-1} with a calculated t_{1/2} = 1.76 min (Stegeman et al. 1993).

Biodegradation: average biodegradation rate of 6.2 mg COD g^{-1} h^{-1} for 97.2% removal (Scow 1982).
Biotransformation: mean bacteria transformation rate constant for all three sites of (2.2 ± 1.7) × 10^{-12} L·organism^{-1}·h^{-1} (Paris & Wolfe 1987; quoted, Steen 1991).

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:
k_{1} = 19.1 h^{-1} (zebrafish, Zok et al. 1991)
k_{2} = 0.21 h^{-1} (carp, Tsuda et al. 1993)

Half-Lives in the Environment:
Biota: t_{1/2} = 3.3 h in carp with excretion rate k = 0.21 h^{-1} (Tsuda et al. 1993).
### TABLE 16.1.3.3.1
Reported vapor pressures of 3-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

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

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<thead>
<tr>
<th>Kahlbaum 1898</th>
<th>Stull 1947</th>
<th>Piacente et al. 1985</th>
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<tr>
<td>static method</td>
<td>summary of literature data</td>
<td>torsion-weighing effusion</td>
</tr>
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<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
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<td>400</td>
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</tr>
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<td>1333</td>
<td>102</td>
</tr>
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<td>110.4</td>
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Overall vapor pressure eq.

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<th>eq. 1</th>
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<tr>
<td>A</td>
<td>8.86 ± 0.10</td>
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</tr>
<tr>
<td>B</td>
<td>3180 ± 40</td>
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</tr>
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</table>

\[\Delta H_v/(kJ \ mol^{-1}) = 60.9 ± 5 \text{ at } 25°C\]
FIGURE 16.1.3.3.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chloroaniline.
16.1.3.4 4-Chloroaniline

Common Name: 4-Chloroaniline  
Synonym: 1-amino-4-chlorobenzene, p-chloroaniline, 4-chlorophenylamine  
Chemical Name: 1-amino-4-chlorobenzene, p-chloroaniline, 4-chloroaniline  
CAS Registry No: 106-47-8  
Molecular Formula: NH₂C₆H₄Cl  
Molecular Weight: 127.572  
Melting Point (°C): 70.5 (Lide 2003)  
Boiling Point (°C): 232.0 (Weast 1982–83; Verschueren 1983; Howard 1989)  
Density (g/cm³ at 20°C): 1.429 (19°C, Weast 1982–83)  
Molar Volume (cm³/mol): 131.1 (calculated-Le Bas method at normal boiling point)  
Dissociation Constant, pKₐ: 3.98 (Perrin 1972; Freitag et al. 1984; quoted, Howard 1989)  
Enthalpy of Fusion, ΔHₙus (kJ/mol): 15.69 (Tsonopoulos & Prausnitz 1971)  
Entropy of Fusion, ΔSₙus (J/mol K): 57.74 (Tsonopoulos & Prausnitz 1971)  
Fugacity Ratio at 25°C (assuming ΔSₙus = 56 J/mol K), F: 0.358 (mp at 70.5°C)  
Water Solubility (g/m³ or mg/L at 25°C): 3000 (Philpot et al. 1940)  
3900 (Kilzer et al. 1979)  
2620 (Schmidt-Bleek et al. 1982; Rott et al. 1982)  
2487 (calculated-group contribution method, Kühne et al. 1995)  
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):  
1.707* (20°C, Knudsen effusion, measured range 10–30°C, Swan & Mack 1925)  
15.19* (extrapolated-regression of tabulated data, temp range 59.3–230.5°C, Stull 1947)  
log (P/mmHg) = [–0.2185 × 12832.8/(T/K)] + 8.461034; temp range 59.3–230.5°C (Antoine eq., Weast 1972–73)  
3.173 (effusion method, DePablo 1976)  
3.33 (extrapolated, Verschueren 1977)  
2.00, 6.67 (20°C, 30°C, quoted, Verschueren 1983)  
0.224 (extrapolated-Antoine eq., Boublik et al. 1984)  
log (P/kPa) = 3.55438 – 521.556/(47.392 + t°C); temp range 90–150°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
1.636* (torsion-weighing effusion, Piacente et al. 1985)
log (P/kPa) = (11.20 ± 0.20) – (4170 ± 60)/(T/K); temp range ~298–360 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)

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

log (P/kPa) = 13.448 – 4736/(T/K), temp range 283–303 K (Antoine eq.—I, Stephenson & Malanowski 1987)

log (PL/kPa) = 7.3489 – 2729/(T/K), temp range 363–505 K (Antoine eq.—II, Stephenson & Malanowski 1987)

3.33, 32.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = –15.3259 – 2.8592 × 10^3/(T/K) + 11.527·log (T/K) – 1.8071 × 10^-2·(T/K) + 7.2359 × 10^-6·(T/K)^2; temp range 343–754 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

1.0840 (calculated-P/C, Howard 1989)

0.0395 (calculated-P/C, Meylan & Howard 1991)

0.1430 (estimated-bond contribution, Meylan & Howard 1991)

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

1.84 (Ichikawa et al. 1969)

1.83 (quoted exptl., Leo et al. 1969, 1971; Hansch & Leo 1985)

1.83 (HPLC-k′ correlation; Carlson et al. 1975)

1.83 (shake flask, Hansch & Leo 1979)

1.57 (HPLC-k’ correlation, Könnemann et al. 1979)

1.83, 20.2 (HPLC-k’ correlation, Hammers et al. 1982)

1.64 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)

1.88 ± 0.02 (HPLC-RV correlation-ALPM; Garst & Wilson 1984)


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

1.83 (RP-HPLC-k’ correlation, Minick et al. 1988)

1.88 ± 0.014 (shake flask/slow-stirring-GC, De Brujin et al. 1989)

1.83 (shake flask, Leahy et al. 1989)

1.80, 1.82 (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.01 (centrifugal partition chromatography CPC-RV correlation, El Tayar et al. 1991)

1.83 (recommended, Sangster 1993)

1.83 (pH 7.4, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

< 1.30 (golden orfe for 3-d exposure, Kört et al. 1978)

3.08 (green algae for 24-h exposure of dry wt. basis, Kört et al. 1978)

2.42 (green algae for 24-h exposure of wet wt. basis, Kört et al. 1978)

< 1.0, 2.41, 3.11 (golden orfe, algae, activated sludge, Freitag et al. 1982)

2.42 (algae Chlorella fusca, wet wt. basis, Geyer et al. 1984)

2.06 (algae Chlorella fusca, calculated-K_{ow}, Geyer et al. 1984)

1.11, 2.42, 2.45 (golden ide, algae, activated sludge, Freitag et al. 1985)

0.91 (zebrafish, Zok et al. 1991)

–0.097–0.23 (carp, Tsuda et al. 1993)

0.91; 1.52, 0.63, 0.88 (quoted; calculated values, Bintein et al. 1993)

2.58 (algae Chlorella fusca, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{oc}:

2.36–2.67 (five Belgium soils, Van Bladel & Moreale 1977)

1.98–3.18 (five German soils, Rott et al. 1982)

3.74 (colloidal org. matter in ground water, Means 1983)

1.86 (calculated-MCI χ, Sabljic 1987)

2.08 (RP-HPLC-k’ correlation, cyanopropyl column, Hodson & Williams 1988)

1.96, 1.86 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
Nitrogen and Sulfur Compounds

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

Volatilization: estimated $t_{1/2} = 6.4$ h from using Henry’s law constant for a model river of 1-m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$\chi = 3$ d in an experimental pond with spiked 4-chloroaniline (Schauerte et al. 1982; 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 NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = (8.3 \pm 0.42) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH} = 83 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH(calc)} = 34.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. in air (Atkinson 1985; Atkinson et al. 1985)

$k_{OH} = 54 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH(calc)} = 83 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = (83 to \sim 44) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295–296 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 42.9$ h$^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.16$ h$^{-1}$ (carp, Tsuda et al. 1993)

$k_1 = 17.74$ h, $k_2 = 0.0465$ h (algae Chlorella fusca, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.6$ h, based on estimated reaction rate with photochemically produced hydroxyl radical of $5 \times 10^5$ radicals/cm$^3$ in atmosphere (Wahner & Zetzsch 1983; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 0.3–3.0$ d in river waters in case of a first order reduction process (Zoeteman et al. 1980);

72.1 mg/L total organic carbon (TOC) degraded to 92% TOC after 5 h illumination with a 250 watt tungsten lamp by photo-Fenton reaction in distilled water (Ruppert et al. 1993).

Groundwater: estimated $t_{1/2} = 30–300$ d in Rhine River (Zoeteman et al. 1980).

Sediment:

Soil:

Biota: $t_{1/2} = 4.3$ h in carp with excretion rate $k = 0.16$ h$^{-1}$ (Tsuda et al. 1993).
### TABLE 16.1.3.4.1
Reported vapor pressures of 4-chloroaniline 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} (1a) \hspace{1cm} (2) \hspace{1cm} (2a) \hspace{1cm} (3) \hspace{1cm} (4)

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\( \Delta H_v / (kJ \ mol^{-1}) = 90.37 \) at 20°C

**FIGURE 16.1.3.4.1** Logarithm of vapor pressure versus reciprocal temperature for 4-chloroaniline.
16.1.3.5 3,4-Dichloroaniline

Common Name: 3,4-Dichloroaniline
Synonym:
Chemical Name: 3,4-dichloroaniline
CAS Registry No: 95-76-1
Molecular Formula: C₆H₅Cl₂N, C₆H₃NH₂Cl₂
Molecular Weight: 162.017
Melting Point (°C):
  72.0 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  272.0 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
  111.7 (calculated-density, Jaworska & Schultz 1993)
  152.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
  2.968, 3.0 (Perrin 1972)
  2.00 (estimated, Wolff & Crossland 1985)
Enthalpy of Fusion, ∆Hₙₙ (kJ/mol):
Entropy of Fusion, ∆Sₙₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₙₙ = 56 J/mol K), F: 0.346 (mp at 72°C)
Water Solubility (g/m³ or mg/L at 25°C):
  92.03 (20°C, Wolff & Crossland 1985)
  93.2; 740 (quoted exper.; calculated-group contribution method, Kühne et al. 1995)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  1.30 (20°C, Wolff & Crossland 1985)
  2.27 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 7.6189 – 3060.03/(T/K); temp range 420–545 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –15.2685 – 3.3857 × 10³/(T/K) + 11.926·log (T/K) – 1.9227 × 10⁻³·(T/K) + 7.4179 × 10⁻⁶·(T/K)²; temp range 345–800 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  2.289 (calculated-P/C)
Octanol/Water Partition Coefficient, log K₀w:
  2.69 (unpublished result, Leo et al. 1971, Hansch & Leo 1979)
  2.12 (HPLC-k' correlation, Könemann et al. 1979)
  2.78 (20°C, shake flask-UV, Briggs 1981)
  2.69, 2.67 (HPLC-k' correlation, Hammers et al. 1982)
  2.62 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
  2.30 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)
  2.14, 2.63 (HPLC-k' correlation, Eadsforth 1986)
  2.69 (shake flask, Log P Database, Hansch & Leo 1987)
  2.68 (recommended, Sangster 1993)
  2.69 (recommended, Hansch et al. 1995)
  2.69 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

1.48 (zebrafish, Zok et al. 1991)
1.48; 2.02, 1.88, 1.75 (fish: quoted; calculated values-$K_{OW}$, Bintein et al. 1993)

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

2.29 (20°C, sorption isotherm-GC, converted from $K_{OM}$ multiplied by 1.724, Briggs 1981)
1.40 (calculated-$K_{OM}$, wet sediment, Wolff & Crossland 1985)
2.29 (Sabljic 1987)
2.05 (soil, quoted, Sabljic 1987)
2.29, 2.08 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
2.29 (calculated-MCI $\chi$, Sabljic et al. 1995)
2.26, 2.39 (RP-HPLC-k’ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

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

Volatilization: first order rate constant $k(\text{calc}) = 5.0 \times 10^{-3} \text{ d}^{-1}$ (Wolff & Crossland 1985).

Photolysis: phototransformation rate constant $k = 0.12$ to $0.20 \text{ d}^{-1}$ (Wolff & Crossland 1985).

Oxidation:

Hydrolysis: not expected to occur (Wolff & Crossland 1985).

Biodegradation:

Biotransformation:

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

$k_1 = 78.5 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Surface water: overall rate of loss predicted from outdoor ponds was calculated based on direct phototransformation, and indirect phototransformation $k = 0.13$ to $0.22 \text{ d}^{-1}$ corresponding to $t_{1/2} = 3.2$ to $5.3 \text{ d}$; the observed rate of loss varied from $0.11$ to $0.17 \text{ d}^{-1}$ corresponding to $t_{1/2} = 4.1$ to $6.3 \text{ d}$ (Wolff & Crossland 1985).
16.1.3.6 o-Toluidine (2-Methylbenzeneamine)

\[
\begin{align*}
\text{NH}_2 & \quad \text{CH}_3 \\
\end{align*}
\]

Common Name: o-Toluidine
Synonym: 2-aminotoluene, o-aminotoluene, 2-methylaniline, 2-methylbenzeneamine
Chemical Name: 2-aminotoluene, o-methylaniline, o-toluidine
CAS Registry No: 95-53-4
Molecular Formula: C₇H₉N, C₆H₄(CH₃)NH₂
Molecular Weight: 107.153
Melting Point (°C):
  \(-14.41\) (Lide 2003)
Boiling Point (°C):
  \(200.3\) (Lide 2003)
Density (g/cm³ at 20°C):
  0.9984, 0.99430 (10, 25°C, Dreisbach 1955, Riddick et al. 1986)
  0.9984 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
  107.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
  132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
  4.40, 4.447, 4.46 (Perrin 1972)
  4.44 (Weast 1982–83)
  4.45 (protonated cation + 1, Dean 1985)
  4.43 (Sangster 1989)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
  56.739, 44.597 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
  7.535 (Dreisbach 1955)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56 \text{ J/mol K}\), F:
Water Solubility (g/m³ or mg/L at 25°C):
  16330 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
  15000 (quoted, Verschueren 1983)
  16300 (calculated-K₆₆₆, Müller & Klein 1992)
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* (48.2°C, static method, measured range 48.2–199.7°C, Kahlbaum 1898)
  42.72* (extrapolated-regression of tabulated data, temp range 44–199.7°C, Stull 1947)
  \[
  \log (P/\text{mmHg}) = 7.60681 – 2033.6/(230 + t/°C) \\
  \] (Antoine eq., Dreisbach & Martin 1949)
  7605* (118.46°C, ebulliometry, measured range 118.46–200.30°C, Dreisbach & Shrader 1949)
  42.26 (calculated by formula, Dreisbach 1955)

\[
\begin{align*}
\text{log (P/mmHg)} & = 7.28896 – 1768.7/(T/K) \times [1 – 473.36/(T/K)] \times 10^6 \times [0.907135 – 6.44774 \times 10^{-4} \times (T/K) + 4.94693 \times 10^{-7} \times (T/K)^2]; \\
\text{temp range:} & \ 300.0–710.0 \text{ K (Cox eq., Chao et al. 1983)} \\
\text{13.33, 40.0} & (20°C, 30°C, quoted, Verschueren 1983) \\
\text{33.96} & (extrapolated-Antoine eq., Boublik et al. 1984)
\end{align*}
\]
\[
\log (P/kPa) = 6.20039 - 1623.158/(186.641 + t/°C); \text{ temp range 118.5–200.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

43.0 (selected lit., Riddick et al. 1986)

\[
\log (P/mmHg) = 6.73171 - 2033.6/(230.0 + t/°C); \text{ temp range: not specified (Antoine eq., Riddick et al. 1986)}
\]

34.18 (extrapolated-Antoine eq., Dean 1985, 1992)

\[
\log (P/mmHg) = 7.08203 - 1627.72/(187.13 + t/°C); \text{ temp range 118–200°C (Antoine eq., Dean 1985, 1992)}
\]

36.46 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/mmHg) = 96.5685 - 6.2643 \times 10^3/(T/K) - 32.265 \cdot \log (T/K) + 1.2361 \times 10^{-2} \cdot (T/K) + 6.2915 \times 10^{-13} \cdot (T/K)^2;
\]

\text{ temp range 249–694 K (vapor pressure eq., Yaws 1994)}

Henry’s Law Constant (Pa·m^3/mol at 25°C):

\[
0.095 \quad \text{(calculated-P/C)}
\]

\[
0.201 \quad \text{(gas stripping-GC, Altschuh et al. 1999)}
\]

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

1.29 (shake flask-UV, Leo et al. 1971)

1.43 (HPLC-’k’ correlation, Carlson et al. 1975)

1.63 (RP-HPLC-RT correlation, Veith et al. 1979a)

1.42 (shake flask-UV at pH 7.5, Martin-Villogre et al. 1986)

1.34 (HPLC-RT correlation, average, Ge et al. 1987)

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

1.32 (recommended, Sangster 1989)

1.44, 1.57 (shake flask, HP:C-RT correlation, Wang et al. 1989)

1.43 (recommended, Sangster 1993)

1.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{oa}\):

Bioconcentration Factor, log BCF:

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

1.24 (calculated-\(K_{ow}\), Kollig 1993)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant \(k = 1 \times 10^4 \text{ M}^{-1} \text{s}^{-1}\) for oxidation by \(\text{RO}_2\) radicals at 30°C in aquatic systems with \(t_\text{1/2} = 0.8\ \text{d}\) (Howard 1972; Hendry et al. 1974; quoted, Mill 1982); rate constant \(k < 2 \times 10^2 \text{ M}^{-1} \text{s}^{-1}\) for oxidation by singlet oxygen at 25°C in aquatic systems with \(t_\text{1/2} > 100\ \text{yr}\) (Foote 1976; Mill 1979; quoted, Mill 1982); photooxidation \(t_\text{1/2} = 62.4 – 3480\ \text{h in water, based on estimated rate constants for reactions of representative aromatic amines with OH and RO}_2\) radicals (Mill & Mabey 1985; quoted, Howard et al. 1991); photooxidation \(t_\text{1/2} = 0.394 – 3.94\ \text{h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)}\).

Biodegradation: decomposition by a soil microflora in > 64 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); aqueous aerobic \(t_\text{1/2} = 24 – 168\ \text{h, based on aqueous aerobic screening test data (Baird et al. 1977; Sasaki 1978; quoted, Howard et al. 1991)}\); average biodegradation \(k = 15.1\ \text{mg COD g}^{-1} \text{h}^{-1}\) for 97.7% removal (Scow 1982); aqueous anaerobic \(t_\text{1/2} = 96 – 672\ \text{h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\).

Biotransformation:
Nitrogen and Sulfur Compounds

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.394 – 3.94$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 1.0$ d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

photooxidation $t_{1/2} = 62.4 – 3480$ h, based on estimated rate constants for reactions of representative aromatic amines with OH and RO$_2$ radicals (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48 – 336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24 – 168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

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<tr>
<th>TABLE 16.1.3.6.1</th>
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<td>Reported vapor pressures of o-toluidine at various temperatures</td>
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</table>

*complete list see ref.
FIGURE 16.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for o-toluidine.
16.1.3.7  \textit{m}-Toluidine (3-Methylbenzeneamine)

\[
\begin{array}{c}
\text{NH}_2 \\
\text{CH}_3
\end{array}
\]

Common Name: \textit{m}-Toluidine  
Synonym: 3-aminotoluene, 3-methylbenzeneamine, 3-methylaniline  
Chemical Name: 3-aminotoluene, \textit{m}-amino-methylbenzene, \textit{m}-methylaniline, \textit{m}-toluidine  
CAS Registry No: 108-44-1  
Molecular Formula: C\textsubscript{6}H\textsubscript{4}(CH\textsubscript{3})NH\textsubscript{2}  
Molecular Weight: 107.153  
Melting Point (°C):  
\(-31.3\) (Lide 2003)  
Boiling Point (°C):  
203.3 (Stull 1947; Weast 1982–83; Lide 2003)  
Density (g/cm\textsuperscript{3} at 20°C):  
0.9889 (Dreisbach 1955; Weast 1982–83)  
Molar Volume (cm\textsuperscript{3}/mol):  
108.4 (20°C, Stephenson & Malanowski 1987)  
132.4 (calculated-Le Bas method at normal boiling point)  
Dissociation Constant, pK\textsubscript{a}:  
4.66, 4.712, 4.72 (Perrin 1972)  
4.73 (Weast 1982–83)  
4.71 (protonated cation + 1, Dean 1985)  
4.70 (Sangster 1989)  
Enthalpy of Vaporization, \Delta H\textsubscript{v} (kJ/mol):  
57.283, 44.848 (25°C, bp, Riddick et al. 1986)  
Enthalpy of Fusion, \Delta H\textsubscript{fus} (kJ/mol):  
7.08 (Dreisbach 1955)  
3.891 (Riddick et al. 1986)  
Entropy of Fusion, \Delta S\textsubscript{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming \Delta S\textsubscript{fus} = 56 J/mol K), F: 1.0  
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):  
15031 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)  
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* (49.8°C, static method, measured range 49.8–203.3°C, Kahlbaum 1898)  
49.54* (extrapolated-regression of tabulated data, temp range 41–203.3°C, Stull 1947)  
7605* (121.77°C, ebulliometry, measured range 121.77-203.34°C, Dreisbach & Shrader 1949)  
36.64 (calculated by formula, Dreisbach 1955)  
19.21 (extrapolated-Antoine eq., Chao et al. 1983)  
25.66 (extrapolated-Antoine eq., Dean 1985, 1992)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = 7.09367 - 1631.43/(183.91 + t/°C); \text{ temp range 122–203°C (Antoine eq., Dean 1985, 1992)} \]

36.0 \hspace{1cm} \text{(quoted lit., Riddick et al. 1986)}

\[ \log \left( \frac{P}{\text{kPa}} \right) = 17.6292 - 3200.9/(T/K) - 3.323 \cdot \log (T/K), \text{ temp range not specified (vapor pressure eq., Riddick et al. 1986)} \]

26.86 \hspace{1cm} \text{(extrapolated-Antoine eq., Stephenson & Malanowski 1987)}

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 7.0317 - 3.2034 \times 10^3/(T/K) + 2.3006 \cdot \log (T/K) - 9.7791 \times 10^{-3} \cdot (T/K) + 4.6824 \times 10^{-6} \cdot (T/K)^2; \text{ temp range 243–709 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa·m³/mol at 25°C):

0.257 \hspace{1cm} \text{(calculated-P/C)}

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

1.40 \hspace{1cm} \text{(shake flask-UV, Fujita et al. 1964)}

1.43 \hspace{1cm} \text{(HPLC-\( k' \) correlation, Carlson et al. 1975)}

1.42 \hspace{1cm} \text{(20°C, shake flask-UV, Briggs 1981)}

1.43 \hspace{1cm} \text{(shake flask, Log P Database, Hansch & Leo 1987)}

1.40 \hspace{1cm} \text{(recommended, Sangster 1989)}

1.49, 1.37 \hspace{1cm} \text{(shake flask, HPLC-RT correlation, Wang et al. 1989)}

1.40 \hspace{1cm} \text{(recommended, Hansch et al. 1995)}

Octanol/Air Partition Coefficient, \( \log K_{oa} \):

Bioconcentration Factor, \( \log BCF \):

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

1.41 \hspace{1cm} \text{(soil, quoted obs. as \( \log K_{om} \), Sabljic 1987)}

1.65 \hspace{1cm} \text{(soil, calculated-MCI \( \chi \), Sabljic et al. 1995)}

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

Volatileization:

Photolysis:

Hydrolysis:

Oxidation: rate constant \( k = 1 \times 10^4 \text{M}^{-1} \text{s}^{-1} \) for oxidation by RO2 radical at 30°C in aquatic systems with \( t_\frac{1}{2} = 0.8 \text{d} \) (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

\( k < 2 \times 10^2 \text{M}^{-1} \text{s}^{-1} \) for oxidation by singlet oxygen at 25°C in aquatic systems with \( t_\frac{1}{2} > 100 \text{yr} \) (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average biodegradation rate of 30.0 mg COD g⁻¹ h⁻¹ for 97.7% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (\( k_u \)) and Elimination (\( k_e \)) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated \( t_\frac{1}{2} = 1.0 \text{d} \) for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
**TABLE 16.1.3.7.1**

Reported vapor pressures of \( m \)-toluidine at various temperatures

<table>
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<th>Kahlbaum 1898</th>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
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<td>ebulliometry</td>
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<tr>
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</tbody>
</table>

*complete list see ref.

**FIGURE 16.1.3.7.1** Logarithm of vapor pressure versus reciprocal temperature for \( m \)-toluidine.
16.1.3.8  *p*-Toluidine (4-Methylbenzeneamine)

![Chemical Structure: NH2 CH3]

Common Name: *p*-Toluidine
Synonym: 4-aminotoluene, 4-methylaniline, 4-methylbenzenamine
Chemical Name: 4-aminotoluene, *p*-amino-methylbenzene, *p*-methylaniline, *p*-toluidine
CAS Registry No: 106-49-0
Molecular Formula: C₆H₄(CH₃)NH₂
Molecular Weight: 107.153
Melting Point (°C): 43.6 (Lide 2003)
Boiling Point (°C): 200.4 (Lide 2003)
Density (g/cm³ at 20°C): 0.9619 (20°C, Weast 1982–83)
1.043 (Verschueren 1983)
Molar Volume (cm³/mol): 132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pHₐ:
5.02, 5.08, 5.084 (Perrin 1972)
5.08 (Weast 1982–83; Sangster 1989)
5.08 (protonated cation + 1, Dean 1985)
5.17 (shake flask-HPLC/UV, Johnson & Westall 1990)
Enthalpy of Vaporization, ∆HV (kJ/mol):
56.195, 44.271 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₕₚ (kJ/mol):
17.32 (Tsonopoulos & Prausnitz 1971)
18.91 (Riddick et al. 1986)
Entropy of Fusion, ∆Sₕₚ (J/mol K):
54.81 (Tsonopoulos & Prausnitz 1971)
57.61 (observed, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ∆Sₕₚ = 56 J/mol K), F: 0.657 (mp at 43.6°C)
Water Solubility (g/m³ or mg/L at 25°C as indicated):
65400 (20–25°C, shake flask-gravimetric, Dehn 1917)
8965 (Seidell 1941, 1952)
7400 (21°C, Verschueren 1983)
6643, 5370 (20°C, shake flask-UV, calculated, Hashimoto et al. 1984)
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* (46.9°C, static method, measured range 46.9–200.4°C, Kahlbaum 1898)
log (P/mmHg) = –2597/(T/K) + 8.366 (isoteniscope method, temp range not specified, Kobe et al. 1941)
46.27* (extrapolated-regression of tabulated data, temper range 42–200.4°C, Stull 1947)
44.70 (calculated from formula, Dreisbach 1955)
log (P/mmHg) = 7.25173 – 1755.0/(201.0 + t°C); temper range 103–330°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/atm) = [–0.2185 × 12428.6/(T/K)] + 8.748585; temper range 42–200.4°C (Antoine eq., Weast 1972–73)
38.13 (calculated-Cox eq., Chao et al. 1983)
\[
\log (P/\text{mmHg}) = \left[1 - 473.445/(T/\text{K})\right] \times 10^8 \{0.915691 - 6.57014 \times 10^{-4} \cdot (T/\text{K}) + 5.11261 \times 10^{-7} \cdot (T/\text{K})^2\}; \text{ temp range 290.0–700.0 K} \text{ (Cox eq., Chao et al. 1983)}
\]
40.17
(calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = \frac{7.26022 - 1758.55/(201.0 + t/°C)}{(-93.44 + T/\text{K})}; \text{ temp range not specified} \text{ (Antoine eq., Dean 1985, 1992)}
\]
45.0
(quoted lit., Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = \frac{18.2818 - 3269.3/(T/\text{K}) - 3.877 \cdot \log (T/\text{K})}{(317–693 \text{ K})}; \text{ temp range not specified} \text{ (vapor pressure eq., Riddick et al. 1986)}
\]
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = \left[1 - 473.445/(T/\text{K})\right] \times 10^8 \{0.915691 - 6.57014 \times 10^{-4} \cdot (T/\text{K}) + 5.11261 \times 10^{-7} \cdot (T/\text{K})^2\}; \text{ temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)}
\]
40.17
(calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = \frac{7.26022 - 1758.55/(201.0 + t/°C)}{(-93.44 + T/\text{K})}; \text{ temp range not specified} \text{ (Antoine eq., Dean 1985, 1992)}
\]
45.0
(quoted lit., Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = \frac{18.2818 - 3269.3/(T/\text{K}) - 3.877 \cdot \log (T/\text{K})}{(317–693 \text{ K})}; \text{ temp range not specified} \text{ (vapor pressure eq., Riddick et al. 1986)}
\]
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = \left[1 - 473.445/(T/\text{K})\right] \times 10^8 \{0.915691 - 6.57014 \times 10^{-4} \cdot (T/\text{K}) + 5.11261 \times 10^{-7} \cdot (T/\text{K})^2\}; \text{ temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)}
\]
40.17
(calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = \frac{7.26022 - 1758.55/(201.0 + t/°C)}{(-93.44 + T/\text{K})}; \text{ temp range not specified} \text{ (Antoine eq., Dean 1985, 1992)}
\]
45.0
(quoted lit., Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = \frac{18.2818 - 3269.3/(T/\text{K}) - 3.877 \cdot \log (T/\text{K})}{(317–693 \text{ K})}; \text{ temp range not specified} \text{ (vapor pressure eq., Riddick et al. 1986)}
\]
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = \left[1 - 473.445/(T/\text{K})\right] \times 10^8 \{0.915691 - 6.57014 \times 10^{-4} \cdot (T/\text{K}) + 5.11261 \times 10^{-7} \cdot (T/\text{K})^2\}; \text{ temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)}
\]
40.17
(calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = \frac{7.26022 - 1758.55/(201.0 + t/°C)}{(-93.44 + T/\text{K})}; \text{ temp range not specified} \text{ (Antoine eq., Dean 1985, 1992)}
\]
45.0
(quoted lit., Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = \frac{18.2818 - 3269.3/(T/\text{K}) - 3.877 \cdot \log (T/\text{K})}{(317–693 \text{ K})}; \text{ temp range not specified} \text{ (vapor pressure eq., Riddick et al. 1986)}
\]
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = \left[1 - 473.445/(T/\text{K})\right] \times 10^8 \{0.915691 - 6.57014 \times 10^{-4} \cdot (T/\text{K}) + 5.11261 \times 10^{-7} \cdot (T/\text{K})^2\}; \text{ temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)}
\]
40.17
(calculated-Antoine eq., Dean 1985, 1992)
\[
\log (P/\text{mmHg}) = \frac{7.26022 - 1758.55/(201.0 + t/°C)}{(-93.44 + T/\text{K})}; \text{ temp range not specified} \text{ (Antoine eq., Dean 1985, 1992)}
\]
45.0
(quoted lit., Riddick et al. 1986)
\[
\log (P/\text{mmHg}) = \frac{18.2818 - 3269.3/(T/\text{K}) - 3.877 \cdot \log (T/\text{K})}{(317–693 \text{ K})}; \text{ temp range not specified} \text{ (vapor pressure eq., Riddick et al. 1986)}
\]
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
Oxidation: rate constant \( k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1} \) for oxidation by \( \text{RO}_2 \) radical at 30°C in aquatic systems with \( t_{1/2} = 0.8 \text{ d} \) (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

\( k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1} \) for oxidation by singlet oxygen at 25°C in aquatic systems with \( t_{1/2} > 100 \text{ yr} \) (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average biodegradation rate of 20 mg COD g\(^{-1}\) h\(^{-1}\) for 97.7% removal (Scow 1982).

Biotransformation:

Biocconcentration, Uptake (\( k_u \)) and Elimination (\( k_e \)) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated \( t_{1/2} = 1.0 \text{ d} \) for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

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<tr>
<th>t/°C</th>
<th>P/Pa</th>
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*complete list see ref.
FIGURE 16.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for \( p \)-toluidine.
16.1.3.9  **N,N’-Dimethylaniline**

![Structure of N,N'-Dimethylaniline]

**Common Name:** N,N’-Dimethylaniline  
**Synonym:** N,N’-dimethylbenzenamine  
**Chemical Name:** N,N’-dimethylaniline  
**CAS Registry No:** 121-69-7  
**Molecular Formula:** C$_8$H$_{11}$N, C$_6$H$_5$N(CH$_3$)$_2$  
**Molecular Weight:** 121.180

- **Melting Point (°C):** 2.42 (Lide 2003)
- **Boiling Point (°C):** 194.0 (Weast 1982–83)  
  194.15 (Lide 2003)
- **Density (g/cm$^3$ at 20°C):** 0.9557 (Weast 1982–83)
- **Molar Volume (cm$^3$/mol):** 154.6 (calculated-Le Bas method at normal boiling point)
- **Dissociation Constant pK:** 5.15 (pK$_{BH^+}$, Riddick et al. 1986)  
  5.10 (Sangster 1993)
- **Enthalpy of Fusion, ΔH$_{fus}$ (kJ/mol):** 11.42 (Tsonopoulos & Prausnitz 1971)
- **Entropy of Fusion, ΔS$_{fus}$ (J/mol K):** 41.46 (Tsonopoulos & Prausnitz 1971)
- **Fugacity Ratio at 25°C (assuming ΔS$_{fus} = 56$ J/mol K), F:** 1.0

**Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):**  
1105 (shake flask-GC, Chiu et al. 1982)  
1540, 1680 (20, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993c)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
106.3 (extrapolated-regression of tabulated data, temp range 20.0–193.1°C, Stull 1947)  
133.3 (29.5°C, Stull 1947)  
83.90 (calculated-Antoine eq., Boublik et al. 1973)  
log (P/atm) = [–0.2185 × 11320.4/(T/K)] + 8.197379; temp range: 29.5–193°C, (Antoine eq., Weast 1972–73)  
68.95 (calculated-Cox eq., Chao et al. 1983)  
log (P/mmHg) = [1 – 466.445/(T/K)] × 10$^4$[0.909397 – 7.07673 × 10$^{-4}$ ± (T/K) + 5.69581 × 10$^{-7}$ ± (T/K)$^2$]; temp range 275.0–685.0 K (Cox eq., Chao et al. 1983)  
84.5 (extrapolated-Antoine eq., Boublík et al. 1984)  
log (P/kPa) = 6.5031 – 1865.084/(211.171 + t°C); temp range 71.02–196.8°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)  
83.91 (extrapolated-Antoine eq., Dean 1985, 1992)  
log (P/mmHg) = 6.91048 – 946.35/(246.68 + t°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)  
670.0 (quoted from Stull 1947, Riddick et al. 1986)  
107.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P$_l$/kPa) = 7.07329 – 2301.63/(–12.001 + T/K); temp range 302–467 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)  
log (P$_l$/kPa) = 6.55663 – 1864.075/(–55.854 + T/K); temp range 363–418 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 2.177 – 3.1095 × 10^(-3)(T/K) + 5.8538 × 10^(-10)(T/K) + 3.5387 × 10^(-7)(T/K)^2;
 temp range 276–687 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol):
11.73 (calculated-P/C)

Octanol/Water Partition Coefficient, log K_{ow}:
2.31 (shake flask-UV, Fujita et al. 1964)
2.62 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
1.66 (shake flask-UV, Leo et al. 1971)
2.29 (shake flask-UV, Yaguzhinskii et al. 1973)
2.30 (shake flask at pH 7, Unger et al. 1978)
2.43 (HPLC-RT correlation, Miyake et al. 1986)
2.28 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.32 (CPC correlation, El Tayar et al. 1991)
2.31 (recommended, Sangster 1993)
2.31 (recommended, Hansch et al. 1995)
2.05 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:
1.99; 2.53; 2.06 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
2.26, 1.89 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.26 (soil, calculated-MCI 1χ, Sabljic et al. 1995)

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 = 1 × 10^{4} M^{-1} s^{-1} for oxidation by RO_{2} radical at 30°C in aquatic systems with t_{1/2} = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
k < 2 × 10^{2} M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with t_{1/2} > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
k_{OH}^{*}(exptl) = (1.48 ± 0.11) × 10^{-10} cm^{3} molecule^{-1} s^{-1}, measured range 278–464 K; k_{O3} = (9.1 ± 1.0) × 10^{-18} cm^{3} molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Atkinson et al. 1987)
k_{OH} = 1.5 × 10^{-10} cm^{3} molecule^{-1} s^{-1} with atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere; k_{O3} = 9.1 × 10^{-18} cm^{3} molecule^{-1} s^{-1} with atmospheric lifetimes of 1.8 d in clean troposphere and 14 h in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)
k_{OH}^{(calc)} = 4.66 × 10^{-10} cm^{3} molecule^{-1} s^{-1}, k_{OH}^{(obs)} = 1.48 × 10^{-10} cm^{3} molecule^{-1} s^{-1}, (SAR structure-activity relationship, Atkinson 1987)
k_{OH}^{(calc)} = 1.78 × 10^{-10} cm^{3} molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aerobic t_{1/2} = 672–4320 h, based on unacclimated aqueous screening test data and anaerobic t_{1/2} = 2880–17280 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:

Half-Lives in the Environment:

Air: atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp.; atmospheric lifetimes of 1.8 d in clean...
troposphere and 14 h in moderately polluted atmosphere, based on the gas-phase reaction with O$_3$ in air at room temp. (Atkinson et al. 1987);
t$_{1/2} = 2.7$–21 h, based on photooxidation half-life in air (Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
Surface water: estimated t$_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
t$_{1/2} = 19.3$–1925 h, based on reaction with singlet oxygen in aqueous solution (Howard et al. 1991)
Groundwater: 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:
Common Name: 2,6-Xylidine
Synonym: 2,6-dimethylaniline, 2,6-dimethylbenzeneamine
Chemical Name: 2,6-dimethylaniline
CAS Registry No: 87-62-7
Molecular Formula: C₈H₁₁N, 2,6-(CH₃)₂C₆H₃NH₂
Molecular Weight: 121.180
Melting Point (°C):
11.20 (Weast 1982–83; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
214.0 (at 739 mm Hg, Weast 1982–83; Verschueren 1983)
215 (Lide 2003)
Density (g/cm³ at 20°C):
0.9842 (Weast 1982–83; Riddick et al. 1986)
Molar Volume (cm³/mol):
123.1 (20°C, calculated-density)
154.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK:
3.95 (pK⁺, Riddick et al. 1986)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
slightly soluble (Dean 1985; Budavari 1989)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
43.03 (extrapolated-regression of tabulated data, temp range 44–217.9°C, Stull 1947)
log (P/atm) = [1–490.795/(T/K)] × 10⁸{(0.926009 – 6.89676 × 10⁻⁸(T/K)) + 5.31053 × 10⁻¹(T/K)²}; temp range: 285.0–720.0 K (Cox eq., Chao et al. 1983)
17.33 (Howard et al. 1986)
670.0 (quoted from Stull 1947, Riddick et al. 1986)
35.99 (calculated-solvatochromic parameters, Banerjee et al. 1990)
Henry’s Law Constant (Pa·m³/mol at 25°C):
17.28 (calculated-P/C from selected value)
Octanol/Water Partition Coefficient, log Kₗₗw:
1.96 (calculated, Verschueren 1983)
1.91 (calculated-CLOGP, Jäckel & Klein 1991)
Octanol/Air Partition Coefficient, log Kₗₗₐ:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₗₗₜₗ:
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

**Volatileization:**

**Photolysis:**

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by $\text{RO}_2$ radical at $30^\circ\text{C}$ in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at $25^\circ\text{C}$ in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 0.33–3.3 \text{ h}$ in air, based on estimated reaction rate constant with OH radical (Atkinson 1987; selected, Howard et al. 1991) and photooxidation $t_{1/2} = 62.4–3480 \text{ h}$ in water, based on reaction rate constants of amine class with $\text{RO}_2$- and OH radicals in water (Güesten et al. 1981; Mill & Mabey 1985; selected, Howard et al. 1991).

**Hydrolysis:** no hydrolyzable group (Howard et al. 1991).

**Biodegradation:**

aqueous aerobic biodegradation $t_{1/2} = 672–4320 \text{ h}$, based on a biological screening study (Baird et al. 1977; selected Howard et al. 1991) and a soil degradation study (Bollag et al. 1978; selected, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 2688–17280 \text{ h}$, based on estimated aqueous biodegradation half-lives (Howard et al. 1991).

**Biotransformation:**

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.33–3.3 \text{ h}$, based on estimated photooxidation half-lives in air from estimated reaction rate constant with OH radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: estimated $t_{1/2} = 2.0 \text{ d}$ for dimethylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$\text{t}_{1/2} = 62.4–3480 \text{ h}$, based on photooxidation half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 1344–8640 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 72–7584 \text{ h}$, based on soil persistence and soil biodegradation studies (Bollag et al. 1978; Medvedev & Davidov 1981; selected, Howard et al. 1991).

Biota:
16.1.3.11 Diphenylamine

Common Name: Diphenylamine
Synonym: N-diphenylamine, N-phenyl aniline, DPA
Chemical Name: N-diphenylamine, diphenylamine
CAS Registry No: 122-39-4
Molecular Formula: C_{12}H_{11}N, C_{6}H_{5}NHC_{6}H_{5}
Molecular Weight: 169.222
Melting Point (°C):
53.2  (Lide 2003)
Boiling Point (°C):
302.0  (Stull 1947; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
1.160  (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
145.9  (20°C calculated-density)
200.3  (calculated-Le Bas method at normal boiling point)
Dissociation Constant, $pK_a$:
0.89  (Perrin 1972)
0.90  (protonated cation + 1, Dean 1985)
0.78  (Sangster 1989)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
17.53  (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
53.56  (Tsonopoulos & Prausnitz 1971)
54.81; 56.5  (exptl., calculated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.529 (mp at 53.2°C)
Water Solubility (g/m³ or mg/L at 25°C as indicated):
150  (20–25°C, shake flask-gravimetric method, Dehn 1917)
308  (Briggs 1981)
48  (20°C, shake flask and membrane filter-fluorophotometric, Hashimoto et al. 1982)
52, 54  (20°C, shake flask and glass fiber filters-fluorophotometric, Hashimoto et al. 1982)
300  (Verschueren 1983)
53  (20°C, Yalkowsky et al. 1987)
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):
0.5682*  (extrapolated-regression of tabulated data, temp range 108.3–302°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 14920.3/(T/K)] + 8.564067; temp range 108.3–302°C (Antoine eq., Weast 1972–73)
log (P/atm) = [1 – 575.114/(T/K)] × 10^{0.936992 – 6.17195 × 10–4·(T/K) + 4.32696 × 10–7·(T/K)^2}; temp range 335.0–670.0 K (Cox eq., Chao et al. 1983)
0.0612  (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 12.704 − 5043.9/(–41.15 + T/K); temp range 298–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 7.15045 − 2778.28/(–35.102 + T/K); temp range 381–575 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.5746 − 2430.7/(–41.15 + T/K); temp range 573–673 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 9.7736 − 3.9008 × 10^{3}/(T/K) + 0.91207·log (T/K) − 5.898 × 10^{3}/(T/K) + 2.3012 × 10^{6}/(T/K)^2; temp range 326–817 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.285 (calculated-P/C, Meylan & Howard 1991)
0.106 (estimated-bond contribution, Meylan & Howard 1991)
0.035 (calculated-P/C from selected values)

Octanol/Water Partition Coefficient, log K_{OW}:
3.23 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)
3.34 (unpublished result, Leo et al. 1971)
3.34, 3.50, 3.72 (unpublished results, Rekker 1977)
2.37 (RP-HPLC-RT correlation, Veith et al. 1979a)
3.45 (Hansch & Leo 1979)
3.42 (shake flask-UV, Briggs 1981)
3.37 (inter-laboratory shake flask average, Eadsforth & Moser 1983)
3.72 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
2.69 (HPLC-RT correlation, average, Ge et al. 1987)
3.42 (shake flask, Log P Database, Hansch & Leo 1987)
3.50 (recommended, Sangster 1989, 1993)
3.70, 3.68 (shake flask, HPLC-RT correlation, Wang et al. 1989)
3.50 (recommended, Hansch et al. 1995)
2.99, 3.13, 3.04, 3.18 (HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
3.35 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
7.64 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
1.48 (fathead minnow, Veith et al. 1979b)
1.48, 2.10 (quoted, calculated-K_{OW}, Mackay 1982)

Sorption Partition Coefficient, log K_{OC}:
2.78 (soption isotherm-GC, converted from K_{OM} organic matter-water in various soils, Briggs 1981)
2.78, 3.28 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
3.30 (calculated-K_{OW}, Kollig 1993)
2.70 (soil, calculated-MCI 1 χ, Sabljic et al. 1995)
2.80, 2.93 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:
Photolysis:
Oxidation: rate constant k = 1 × 10^4 M⁻¹ s⁻¹ for oxidation by RO₂ radical at 30°C in aquatic systems with t_{1/2} = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);
k < 2 × 10^2 M⁻¹ s⁻¹ for oxidation by singlet oxygen at 25°C in aquatic systems with t_{1/2} > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982);
photooxidation t_{1/2} = 31–1740 h in water, based on photooxidation rate constants with OH and RO₂ radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991);
photooxidation t_{1/2} = 0.247–2.47 h, based on estimated rate data for the reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991).
Hydrolysis: rate constant k = 1.2 × 10¹⁰ L mol⁻¹ s⁻¹ for reactions with hydroxyl radical in aqueous solution, (Buxton et al. 1986; quoted, Armbrust 2000);
measured hydroxy radical rate constant k = 4.9 × 10¹³ M⁻¹·h⁻¹ (Armbrust 2000)
Biodegradation: aqueous aerobic t_{1/2} = 168–672 h, based on estimated aqueous aerobic biodegradation screening test data (Malaney 1960; quoted, Howard et al. 1991);
aqueous anaerobic $t_{1/2} = 672–2688$ 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: photooxidation $t_{1/2} = 0.247–2.47$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 31–1740$ h in water, based on photooxidation rate constants with OH and RO$_2$ radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991); $t_{1/2} = 31–672$ h, based on estimated unacclimated aqueous aerobic degradation half-life and photooxidation half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 336–1344$ 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:

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**TABLE 16.1.3.11.1**
Reported vapor pressures of diphenylamine at various temperatures

<table>
<thead>
<tr>
<th>Stull 1947 summary of literature data</th>
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<tbody>
<tr>
<td>t/$^\circ$C</td>
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<tr>
<td>108.3</td>
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<td>141.7</td>
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<td>157.0</td>
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<td>175.2</td>
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<td>194.3</td>
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<td>247.5</td>
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<td>274.1</td>
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<tr>
<td>302.0</td>
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<tr>
<td>mp/$^\circ$C</td>
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</tbody>
</table>
FIGURE 16.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylamine.
16.1.3.12 Benzidine

Common Name: Benzidine
Synonym: \( p,p^{\prime}\)-bianiline, 4,4'-diaminobiphenyl, 4,4'-biphenyldiamine, (1,1'-biphenyl)-4,4'-diamine
Chemical Name: \( p\)-benzidine
CAS Registry No: 92-87-5
Molecular Formula: \( \text{C}_{12}\text{H}_{12}\text{N}_{2}, \text{NH}_2\text{C}_6\text{H}_4\text{C}_6\text{H}_4\text{NH}_2 \)
Molecular Weight: 184.236
Melting Point (°C):
- 128 (Weast 1982–83)
- 120 (Lide 2003)
Boiling Point (°C):
- 400 (Weast 1982–83)
- 401 (Lide 2003)
Density (g/cm³ at 20°C):
- 1.250 (Verschueren 1983)
Molar Volume (cm³/mol):
- 213.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, \( \text{pK}_a \):
- 4.66 (\( \text{pK}_1 \)), 3.57 (\( \text{pK}_2 \)) (30°C, Perrin 1965; quoted, Mabey et al. 1982; Howard 1989)
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), \( F \): 0.117 (mp at 120°C)
Water Solubility (g/m³ or mg/L at 25°C as indicated):
- 400 (12°C, Verschueren 1977, 1983)
- 520 (Shriner et al. 1978)
- 360 (24°C at pH 5.9, shake flask-LSC, Means et al. 1980)
- 276 (20°C, Schmidt-Bleek et al. 1982)
- 359 (Gerstl & Helling 1987)
Vapor Pressure (Pa at 25°C):
- 0.724 (calculated-Trouton’s rule, Mabey et al. 1982)
- 1.0 × 10⁻⁶ (20°C, Schmidt-Bleek et al. 1982)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
- 3.93 × 10⁻⁶ (estimated, Hine & Mookerjee 1975)
- 0.0394 (calculated-P/C at 12°C, Mabey et al. 1982)
- 4.60 × 10⁻⁷ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
- 1.34 (shake flask, Korenman 1971)
- 1.34 (recommended, Sangster 1993)
- 1.34 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF:
- 1.74, 2.66, 2.81, 3.4 (fish, mosquitoes, snail, algae; Lu et al. 1977)
- 1.60 (bluegills, USEPA 1980; quoted, Howard 1989)
- 1.00 (microorganisms-water, calculated-\( K_{\text{OW}} \), Mabey et al. 1982)
1.90, 2.93, 3.08 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log $K_{OC}$:
- 1.66 (soil/sediment, equilibrium sorption isotherm by shake flask-LSC at pH 5.9, Means et al. 1980)
- 1.02 (sediment-water, calculated-$K_{OC}$, Mabey et al. 1982)
- 5.95; 5.68; 5.35; 5.91 (Russell soil; Chalmers soil; Kokomo soil; Milford soil, Graveel et al. 1986)
- 3.00 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 3.46, 3.44 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 1.26 (calculated-$K_{OC}$, Kollig 1993)
- 3.46 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7$ M$^{-1}$ h$^{-1}$ and for peroxy radical of $1.1 \times 10^8$ M$^{-1}$ h$^{-1}$ at 25°C (Mabey et al. 1982);

- photooxidation $t_{1/2} = 0.312–3.12$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 48–192$ h, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

- overall biodegradation $t_{1/2} = 76$ d, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989);

- aqueous aerobic $t_{1/2} = 192–768$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation of $1 \times 10^{-10}$ mL·cell$^{-1}$·h$^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.312–3.12$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

- estimated $t_{1/2} \sim 1$ d for the reaction with hydroxyl radical and ozone (Howard 1989);

- atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} \sim 1$ d for the reaction with radicals and redox reactions with naturally occurring cations, etc. and perhaps with photodegradation (Howard 1989);

- $t_{1/2} = 31.2–192$ h, based on estimated photooxidation half-life in water and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 96–484$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10$ d in soil (USEPA 1979; quoted, Ryan et al. 1988);

- $t_{1/2} = 48–192$ h, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

- overall biodegradation $t_{1/2} = 76$ d, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989).

Biota: depuration $t_{1/2} \sim 7$ d from bluegills (Lu et al. 1977; quoted, Howard 1989).
### 16.1.3.13 3,3'-Dichlorobenzidine

![Chemical Structure](image)

- **Common Name:** 3,3'-Dichlorobenzidine
- **Synonym:** 3,3'-dichloro-4,4'-diamino(1,1'-biphenyl), DCB
- **Chemical Name:** 3,3'-dichlorobenzidine
- **CAS Registry No:** 91-94-1
- **Molecular Formula:** C_{12}H_{10}Cl_{2}N_{2}, NH_{2}C_{6}H_{3}(Cl)C_{6}H_{3}(Cl)NH_{2}
- **Molecular Weight:** 253.126
- **Melting Point (°C):** 132.5 (Lide 2003)
- **Boiling Point (°C):**
- **Density (g/cm³ at 20°C):** 254.8 (calculated-Le Bas method at normal boiling point)
- **Molar Volume (cm³/mol):**
- **Dissociation Constant, pKₐ:** 11.7 (Kollig 1993)
- **Enthalpy of Fusion, ∆Hₜₚ (kJ/mol):**
- **Entropy of Fusion, ∆Sₜₚ (J/mol K):**
- **Fugacity Ratio at 25°C (assuming ∆Sₜₚ = 56 J/mol K), F:** 0.0882 (mp at 132.5°C)
- **Water Solubility (g/m³ or mg/L at 25°C or as indicated):**
  - 4.00 (22°C, as dihydrochloride, Banerjee et al. 1978)
  - 3.99 (22°C, at pH 6.9 as DCB·2HCl, quoted, Verschueren 1983)
  - 3.11 (shake flask-UV/LSC, Banerjee et al. 1980)
- **Vapor Pressure (Pa at 25°C):** 0.00133 (estimated, Mabey et al. 1982)
- **Henry’s Law Constant (Pa·m³/mol at 25°C):** 0.0811 (calculated-P/C, Mabey et al. 1982)
- **Octanol/Water Partition Coefficient, log K_{OW}:**
  - 3.02 (calculated as per Leo et al.1971)
  - 3.51 (23°C, shake flask, Banerjee et al. 1980)
  - 3.35 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
  - 3.51 (recommended, Sangster 1993)
  - 3.51 (recommended, Hansch et al. 1995)
- **Octanol/Air Partition Coefficient, log K_{OA}:**
- **Bioconcentration Factor, log BCF:**
  - 2.70 (bluegill sunfish, Appleton & Sikka 1980)
  - 2.97 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
  - 2.79, 2.97, 3.49 (fish, algae, activated sludge, Freitag et al. 1985)
- **Sorption Partition Coefficient, log K_{OC}:**
  - 3.19 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
  - 4.35, 3.87 (soil: quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
  - 3.30 (calculated-K_{OW}, Kollig 1993)
  - 4.35 (soil, calculated-MCI ¹χ, Sabljic et al. 1995)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volutilization:

Photolysis:
- direct aqueous photolysis rate constant $k = 2.1 \times 10^{-6}$ h$^{-1}$ in summer at 40°N latitude (Mabey et al. 1982);
- both aqueous and atmospheric photolysis $t_{1/2} = 0.025$–0.075 h, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Callahan et al. 1979; Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7$ M$^{-1}$ h$^{-1}$ and for peroxy radical $k < 4 \times 10^7$ M$^{-1}$ h$^{-1}$ at 25°C (Mabey et al. 1982);
- photooxidation $t_{1/2} = 31.2$ – 1740 h in water, based on estimated rate constants for reactions with OH and RO$_2$ radicals in water (Mill & Mabey 1985; quoted, Howard et al. 1991);
- photooxidation $t_{1/2} = 0.905$ – 9.05 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 672$ – 4320 h, based on lake die-away study test data (Appleton et al. 1978; quoted, Howard et al. 1991) and a soil die-away test (Boyd 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: rate constant for bacterial transformation $k = 3 \times 10^{-12}$ mL·cell$^{-1}$·h$^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.905$ – 9.05 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- estimated $t_{1/2} \sim 1$ d for the reaction with hydroxyl radical and ozone (Howard 1989);
- atmospheric transformation lifetime by photolysis was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 0.025$ – 0.075 h, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, 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: $t_{1/2} = 30$ min by suspended microcrystalline clays may be considered the most important fate process in the aquatic environment (Callahan et al. 1979).

Soil: $t_{1/2} = 672$ – 4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
16.1.3.14  N,N’-Bianiline

Common Name: N,N’-Bianiline
Synonym: 1,2-diphenylhydrazine, hydrazobenzene
Chemical Name: 1,2-diphenylhydrazine, hydrazobenzene
CAS Registry No: 122-66-7
Molecular Formula: C_{12}H_{12}N_{2}, C_{6}H_{5}NHNHC_{6}H_{5}
Molecular Weight: 184.236

Melting Point (°C):
131 (Weast 1982–83; Lide 2003)

Boiling Point (°C):
293 (as azobenzene, IARC 1975)
1.158 (16°C, Weast 1982–83)

Molar Volume (cm³/mol):
213.0 (calculated-Le Bas method at normal boiling point)

Dissociation constant pK₆:
13.2 (Kollig 1993)

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: 0.0912 (mp at 131°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.252 (20°C, as azobenzene, Takagishi et al. 1968)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00347 (quoted, Mabey et al. 1982)
log (P/mmHg) = 16.8982 – 5.0039 × 10³/(T/K) – 9.9629 × 10⁻³·(T/K) + 4.2938 × 10⁻⁶·(T/K)²;
temp range 404–573 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
3.45 × 10⁻⁴ (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
3.82 (shake flask-UV as for azobenzene, Fujita et al. 1964)
3.03 (calculated as per Leo et al. 1971, Callahan et al. 1979)
2.94 (shake flask, Hansch & Leo 1979; 1987)
2.94 (recommended, Sangster 1993)
2.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.46 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.62 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.40 (calculated-K_{OW}, Kollig 1993)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatileization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen k < 4 × 10⁷ M⁻¹ h⁻¹ and for peroxy radical, k < 1 × 10⁹ M⁻¹ h⁻¹ at 25°C (Mabey et al. 1982);

photooxidation t½ = 31 – 1740 h, based on photooxidation rate constants with OH and RO₂ radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation t½ = 0.3 – 3.0 h in air, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic t½ = 672 – 4320 h, based on acclimated aerobic aqueous screening test data (Malaney 1960; quoted, Howard et al. 1991); aqueous anaerobic t½ = 2880 – 17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: bacterial transformation k = 1 × 10⁻¹⁰ mL·cell⁻¹·h⁻¹ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation t½ = 0.3 – 3.0 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).


Groundwater: t½ = 1344 – 8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: t½ = 672 – 4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
16.1.3.15 α-Naphthylamine (1-Aminonaphthalene)

Common Name: 1-Naphthylamine
Synonym: 1-naphthalenamine, α-naphthylamine, 1-NA, 1-aminonaphthalene, naphthalidine
Chemical Name: 1-naphthalenamine
CAS Registry No: 134-32-7
Molecular Formula: C_{10}H_{7}N\textsubscript{2}
Molecular Weight: 143.185
Melting Point (°C):
- 49.2 (Lide 2003)
Boiling Point (°C):
- 300.7 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
- 1.1229 (25°C, Weast 1982–8)
- 1.123 (Dean 1985)
Molar Volume (cm\textsuperscript{3}/mol):
- 161.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK\textsubscript{a}:
- 3.92 (Sangster 1993)
Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):
- 14.23 ± 0.105 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):
- 44.35 ± 3.35 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), F: 0.579 (mp at 49.2°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 1700 (Verschueren 1983)
- 590 parts in water (Budavari 1989)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.803 (extrapolated-regression of tabulated data, temp range 104.3–300.8°C, Stull 1947)
  \[ \log (P/\text{mmHg}) = [1 - 0.2185 \times 14529.5/(T/K)] + 8.29900; \text{ temp range 104.3–300.8°C} \]
- 0.557 (extrapolated-Cox eq., Chao et al. 1983)
  \[ \log (P/\text{atm}) = [1 - 574.066/(T/K)] \times 10^{0.822931 - 2.94554 \times 10^{-4} \times (T/K) + 2.19845 \times 10^{-7} \times (T/K)^2}; \text{ temp range: 325.0–645.0 K} \]
- 0.446 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)
  \[ \log (P/\text{kPa}) = 6.88407 - 2570.55/(-46.989 + T/K); \text{ temp range 377–574 K} \]
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
- 6.197 (gas stripping-GC, Altschuh et al. 1999)
Octanol/Water Partition Coefficient, log \(K_{\text{ ow}}\):
- 2.23 (Leo et al. 1969)
- 2.25 (shake flask, Hansch & Leo 1979)
- 2.27 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
- 2.33 (HPLC-k′ correlation, Minick et al. 1988)
- 2.25 (recommended, Sangster 1993)
- 2.25 (recommended, Hansch et al. 1995)
- 2.34 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:
- 3.58, 3.43, 3.50 (Milford soil, Morocco soil, Oakville soil, Graveel et al. 1986)
- 2.63, 2.68, 3.15 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
- 3.51, 3.48 (soil, quoted exptl., calculated-MCI $\chi$, Meylan et al. 1992)
- 3.51 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.0–2.65 (5 soils, pH 2.8–7.4, batch equilibrium-sorption isotherm, Li et al. 2000)

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

Volatileization:
- Volatilization: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{s}^{-1}$ for oxidation by RO$_2$ radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);
- rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);
- atmospheric $t_{1/2} = 0.292–2.92 \text{ h}$, based on estimated rate constants for the reaction with OH radical in air and aqueous photooxidation $t_{1/2} = 62.4–3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO$_2$ radicals in aqueous solution (Howard et al. 1991);
- photooxidation $t_{1/2} = 0.08–0.13 \text{ h}$ under sunlight and $t_{1/2} = 0.25–9.1 \text{ h}$ under UV light when adsorbed on silica;
- $t_{1/2} = 0.10–0.15 \text{ h}$ under sunlight and $t_{1/2} = 0.15–10.5 \text{ h}$ under UV light when adsorbed on alumina on the TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:
- Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672–4320 \text{ h}$ and aqueous anaerobic biodegradation $t_{1/2} = 2688–17280 \text{ h}$, based on slow biodegradation observed in aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

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

Half-Lives in the Environment:
- Air: $t_{1/2} = 0.292–2.92 \text{ h}$, based on estimated photooxidation half-life in air (Howard et al. 1991).
- Surface water: $t_{1/2} = 0.624–3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO$_2$ radicals in aqueous solutions (Howard et al. 1991).
- Groundwater: $t_{1/2} = 1344–8640 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).
- Sediment:
- Soil: $t_{1/2} = 672–4320 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).
- Biota:
16.1.3.16 β-Naphthylamine (2-Aminonaphthalene)

Common Name: 2-Naphthylamine
Synonym: 2-naphthalenamine, β-naphthylamine, 2-NA, 2-aminonaphthalene, naphthalidine
Chemical Name: 2-naphthalenamine
CAS Registry No: 91-59-8
Molecular Formula: C10H7NH2
Molecular Weight: 143.185
Melting Point (°C):
113 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
306.2 (Lide 2003)
Density (g/cm³):
1.0614 (at 98°C, Weast 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
161.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
4.15 (Sangster 1993)
Enthalpy of Fusion, ΔH₉₋₀ (kJ/mol):
21.97 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS₉₋₀ (J/mol K):
57.32 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS₉₋₀ = 56 J/mol K), F: 0.137 (mp at 113°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
6.40 (18°C, Ciusa 1922; quoted, Tsonopoulos & Prausnitz 1971)
0.19 (18–20°C, Neish 1948; quoted, Tsonopoulos & Prausnitz 1971)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.634 (extrapolated-regression of tabulated data, temp range 108–306.1°C, Stull 1947)
log (P/atm) = [–0.2185 × 14679.6/(T/K)] + 8.435133; temp range 108–306.1°C (Antoine eq., Weast 1972–73)
0.369 (extrapolated-Cox eq., Chao et al. 1983)
log (P/atm) = [1 – 579.422/(T/K)] × 10^4(0.860256 – 4.44286 × 10^{-4}(T/K) + 3.71453 × 10^{-7}(T/K)^2); temp range: 385.0–645.0 K (Cox eq., Chao et al. 1983)
0.035 (Howard et al. 1986)
0.035 (interpolated, solid, Antoine eq., Stephenson & Malanowski 1987)
0.362 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)
log (P_kPa) = 8.4859 – 3859/(T/K), temp range: 283–323 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_kPa) = 6.88978 – 2604.31/(–46.068 + T/K), temp range 388–579 K (Antoine eq.-II, Stephenson & Malanowski 1987)
0.340 (calculated-solvatochromic parameters, Banerjee et al. 1990)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
2.28 (shake flask, Hansch & Leo 1979)
2.26 (20°C, shake flask, Korenman & Polumestnaya, 1982)
2.40 (calculated-UNIFAC activity coeff., Campbell & Luthy 1985)
2.40 (shake flask-AS, pH 7.5, Martin-Villodre et al. 1986)
2.34 (recommended, Sangster 1993)
2.28 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

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

1.77 (calculated-$K_{OW}$, Kollig 1993)

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

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO$_2$ radicals at 30°C in aquatic systems with $t_\text{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mil1 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_\text{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_\text{1/2} = 0.30–2.90 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

aqueous photooxidation $t_\text{1/2} = 62–3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO$_2$ radicals in aqueous solution (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_\text{1/2} = 0.05–0.14 \text{ h}$ under sunlight and 0.20–10.0 h under UV light when adsorbed on silica and $t_\text{1/2} = 0.16–0.19 \text{ h}$ under sunlight and $t_\text{1/2} = 0.22–10.8 \text{ h}$ under UV light when adsorbed on alumina TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_\text{1/2} = 672–4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1979) and unacclimated soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_\text{1/2} = 2880–17280 \text{ h}$, 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: photooxidation $t_\text{1/2} = 0.30–2.90 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_\text{1/2} = 62.0–3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO$_2$ radicals in aqueous solutions (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_\text{1/2} = 1344–8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_\text{1/2} = 672–4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1991) and unacclimated aerobic soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1981).

Biota:
16.1.3.17 2-Nitroaniline

Common Name: 2-Nitroaniline
Synonym: 1-amino-2-nitrobenzene, o-aminonitrobenzene, o-nitroaniline, 2-nitrophenylamine, 2-nitrobenzeneamine
Chemical Name: 1-amino-2-nitrobenzene, o-nitroaniline, 2-nitroaniline
CAS Registry No: 88-74-4
Molecular Formula: C₆H₆N₂O₂, C₆H₄NH₂NO₂
Molecular Weight: 138.124
Melting Point (°C):
71.0 (Lide 2003)
Boiling Point (°C):
284 (Lide 2003)
Density (g/cm³ at 20°C):
1.442 (15°C, Weast 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
138.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:

Enthalpy of Fusion, ΔHₚᵤₛ (kJ/mol):
16.11 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔSₚᵤₛ (J/mol K):
46.86 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔSₚᵤₛ = 56 J/mol K), F: 0.354 (mp at 71.0°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1212, 2423 (25, 40°C, synthetic method-shake flask-titration, Collet & Johnson 1926)
1740 (calculated-Kₗₒ₆, Yalkowsky & Morozowich 1980)
1260 (Verschueren 1983)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/mmHg) = 8.81842 – 3336.52/(T/K); measured range 150–215°C (isoteniscope, Berliner & May 1925)
log (P/mmHg) = 9.55950 – 4037.7/(T/K); measured range 190–250°C (isoteniscope, Berliner & May 1925)
0.620 (extrapolated-regression of tabulated data, temp range 104–284.5°C, Stull 1947)
0.072 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)
log (P/mmHg) = 12.50 – 4701/(T/K), temp range 0–50°C (Knudsen effusion method, Hoyer & Peperle 1958)
log (P/mmHg) = -0.2185 × 15284.0/(T/K) + 8.686838; temp range 104–284.5°C (Antoine eq., Weast 1972–73)
< 13.3 (30°C, Verschueren 1983)
0.650 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 8.8684 – 3336.5/(T/K); temp range 150–260°C (Antoine eq., Dean 1985, 1992)
log (Pₗ/kPa) = 11.625 – 4701/(T/K); temp range 273–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (Pₗ/kPa) = 11.3629 – 7444.3/(240.83 + T/K); temp range 423–553 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = -112.5774 – 1.5945 × 10⁹/(T/K) + 54.577·log (T/K) – 7.6775 × 10⁻²·(T/K) + 3.6152 × 10⁻⁵·(T/K)²;
temp range 345–558 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₗₒ₆:
1.44 (shake flask-UV, Fujita et al. 1964)
1.83 (shake flask-UV, Hansch & Anderson 1967)
1.62 (HPLC-RT correlation, Carlson et al. 1975)
1.81 (Hansch & Leo 1979)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

0.91; 1.49, 0.55, 0.83 (quoted exptl.; calculated values-$K_{OW}$, Bintein et al. 1993)

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

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

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 1.4$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
16.1.3.18 4-Nitroaniline

Common Name: 4-Nitroaniline
Synonym: 1-amino-4-nitrobenzene, p-aminonitrobenzene, p-nitroaniline, 4-nitrobenzenamine, 4-nitrophenylamine
Chemical Name: 1-amino-4-nitrobenzene, p-nitroaniline, 4-nitroaniline
CAS Registry No: 100-01-6
Molecular Formula: C₆H₆N₂O₂, C₆H₄NH₂NO₂
Molecular Weight: 138.124
Melting Point (°C): 147.5 (Lide 2003)
Boiling Point (°C): 332 (Lide 2003)
Density (g/cm³ at 20°C):
  1.424 (Weast 1982–83; Verschueren 1983)
  1.4370 (14°C, Dean 1985)
Molar Volume (cm³/mol):
  138.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH_fus (kJ/mol):
  21.09 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_fus (J/mol K):
  50.21 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.0628 (mp at 147.5°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  568, 1157 (25, 40°C, synthetic method-shake flask-titration, Collet & Johnson 1926)
  728 (30°C, shake flask-interferometry, Gross et al. 1931)
  603 (calculated-K_ow, Yalkowsky & Morozowich 1980)
  380 (20°C, shake flask-membrane filter-fluorophotometry, Hashimoto et al. 1982)
  390, 400 (20°C, shake flask-glass fiber filters-fluorophotometry, Hashimoto et al. 1982)
  800; 22000 (19°C, 100°C, Verschueren 1983)
  800 (Dean 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  log (P/mmHg) = 9.55950 – 4037.7/(T/K); measured range 190–250°C (isoteniscope, Berliner & May 1925)
  0.035 (extrapolated-regression of tabulated data, temp range 142.4–336°C, Stull 1947)
  log (P/mmHg) = 13.69 – 5707/(T/K); temp range 30–90°C, (Knudsen effusion method, Hoyer & Peperle 1958)
  log (P/mmHg) = [-0.2185 × 17220.2/(T/K)] + 9.041879; temp range 142.4–336°C (Antoine eq., Weast 1972–73)
  0.200, 0.933 (20°C, 30°C, Verschueren 1983)
  0.014 (extrapolated-Antoine eq., Dean 1985)
  log (P/mmHg) = 9.5595 – 4039.73/(T/K); temp range 190–260°C (Antoine eq., Dean 1985, 1992)
  log (P/kPa) = 11.1109 – 5093/(T/K); temp range 346–366 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 8.7988 – 4071.3/(T/K); temp range 473–538 K (liquid, Antoine eq.-II., Stephenson & Malanowski 1987)
  log (P/mmHg) = 56.1642 – 5.3655 × 10³/(T/K) –17.958-log (T/K) + 9.092 × 10⁻³-(T/K) + 7.0305 × 10⁻¹⁰·(T/K)²; temp range 421–609 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 1.39 (shake flask-UV, Fujita et al. 1964; Hansch & Leo 1979)
- 0.59 (calculated-activity coeff. $\gamma$ from UNIFAC, Campbell & Luthy 1985)
- 1.16 (HPLC-$k'$ correlation, Deneer et al. 1987)
- 1.10 (calculated-linear extrapolation exptl. values of log $k$ at various solvent compositions, Deneer et al. 1987)
- 1.15 (HPLC-RT correlation, Wang et al. 1989)
- 1.51, 1.36 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
- 1.30 (CPC-RV correlation, Tsai et al. 1991)
- 1.35 (CPC-RV correlation, El Tayar et al. 1991)
- 1.39 ± 0.14, 0.75 ± 0.48 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-$k'$ correlation, Cichna et al. 1995)
- 1.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:
- 2.26; 2.66; 2.12 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 0.64; 1.25, −0.18, 0.41 (quoted exptl.; calculated values-$K_{OW}$, Bintein et al. 1993)
- 2.16, 2.22, 2.19 (RP-HPLC-$k'$ correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.86, 1.84 (RP-HPLC-$k'$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

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

Half-Lives in the Environment:
- Surface water: estimated $t_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
16.1.4 NITROAROMATIC COMPOUNDS

16.1.4.1 Nitrobenzene

Common Name: Nitrobenzene
Synonym: nitrobenzol, oil of mirbane
Chemical Name: nitrobenzene
CAS Registry No: 98-95-3
Molecular Formula: C₆H₅NO₂
Molecular Weight: 123.110

Melting Point (°C):
5.7 (Stull 1947; Dreisbach 1955; Weast 1982–83; Howard 1989; Lide 2003)

Boiling Point (°C):
210.8 (Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
1.2032, 1.1982 (20°C, 25°C, Dreisbach 1955)
1.2036 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
102.0 (calculated from density, Rohrschneider 1973; Chiou 1985)
112.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
55.186, 43.421 (25°C, bp, Dreisbach 1961)
55.013, 40.769 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
11.59 (Dreisbach 1955)
12.13 (Tsonopoulos & Prausnitz 1971)
11.63 (Riddick et al. 1986)

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
43.51 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), 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):
1780, 2050 (15, 30°C, shake flask-interferometry, Gross et al. 1931)
2060* (30°C, shake flask-interferometry and titration, measured range 0–60°C, Vermillion et al. 1941)
1204 (shake flask-centrifuge, Booth & Everson 1948)
1930 (Seidell 1941)
2018 (shake flask-interferometry, Donahue & Bartell 1952)
1950 (Deno & Berkheimer 1960)
2259 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
2060 (Hansch et al. 1968)
1900 (20°C, Verschueren 1977, 1983)
2093 (shake flask-LSC, Banerjee et al. 1980)
2090 (shake flask-radioactive analysis, Veith et al. 1980)
2043 (20–27°C, shake flask-GC, Chiou 1985)
1900 (20°C, Riddick et al. 1986; quoted, Howard 1989)
1930* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 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):

133.3* (53.1°C, static-manometer, measured range 53.1–208.3°C, Kahlbaum 1898)
38.80 (saturated vapor density-gas saturation, Puck & Wise 1946)
42.06* (extrapolated-regression of tabulated data, temp range 44.4–210.6°C, Stull 1947)
10063* (134.1°C, ebulliometry, measured range 134.1–210.629°C, Brown 1952)
37.86 (calculated by formula, Dreisbach 1955; quoted, Hine & Mookerjee 1975)

log (P/mmHg) = 7.08283 – 1722.2/(199.0 + t/°C); temp range 108–300°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = 7.545 – 2064/(t/°C + 230); temp range 6.09–23.14°C (gas saturation, Lynch & Wilke 1960)
80.0 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
34.60 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.11562 – 1746.585/(201.783 + t/°C), temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
20.00 (20°C, Verschueren 1977, 1983)
28.37 (calculated-bp, Mackay et al. 1982)
34.36 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.23424 – 1741.779/(201.257 + t/°C); temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 4.06596 – 323.457/(−58.276 + t/°C); temp range 239–291°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
34.63 (extrapolated-Antoine eq., Dean 1985; 1992)

log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
37.0 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.670 – 2064.0/(230.0 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
37.65 (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.22069 – 1732.222/(−72.886 + T/K); temp range 407–484 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.6699 – 2064/(−43.15 + T/K); temp range 279–296 K (Antoine eq.-II, Stephenson & Malanowski 1987)
33.33 (Howard et al. 1986)
log (P/mmHg) = −54.4937 – 2.1123 × 10³/(T/K) + 29.321 log (T/K) – 4.4839 × 10⁻² (T/K) + 2.0162 × 10⁻⁵ (T/K)²; temp range 279–719 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
2.367, 4.51, 4.723 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1.327 (calculated-P/C, Mabey et al. 1982)
2.472 (estimated, Lyman et al. 1982)
5.06 (calculated-molecular structure, Russell et al. 1992)
0.868 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.74 (Neely et al. 1974)
1.85, 1.84 (Hansch & Leo 1979)
1.82 (HPLC-RT correlation, Veith et al. 1979a)
1.83 (shake flask-LSC, Banerjee et al. 1980)
1.98, 1.78 (HPLC-k’ correlation, McDuffie 1981)
1.85 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982;)
1.88 (shake flask-UV, Unger & Chiang 1981)
1.99 (RP-HPLC-k’ correlation, Miyake & Terada 1982)
1.83, 1.84 (calculated-activity coeff. γ from UNIFAC, octanol and water solubility considered; calculated-activity coeff. γ from UNIFAC, octanol and water solubility not considered, Arbuckle 1983)
1.85, 1.88 (lit. values, Verschueren 1983)
Nitrogen and Sulfur Compounds

1.83 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.84 (calculated-activity coefficient \( \gamma \) from UNIFAC, Campbell & Luthy 1985)
1.87 (Lu et al. 1986)
1.85 (RP-HPLC-k' correlation, Minick et al. 1988)
1.89 (HPLC-k' correlation, Deneer et al. 1987)
1.84 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)
1.70 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.828 ± 0.001 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
1.85 (recommended, Sangster 1989, 1993)
1.836 ± 0.051; 1.828 ± 0.001 (average values, stir-flask method by BRE; by RITOX, Brooke et al. 1990)
1.83, 1.85, 1.88 (CPC-retention volume correlation; Gluck & Martin 1990)
1.94, 2.25 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
1.57 (shake flask-UV, Nakagawa et al. 1992)
1.85 (shake flask-UV, Alcron et al. 1993)
1.85 (recommended, Hansch et al. 1995)
2.25, 2.12, 2.20, 2.23 (HPLC-k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
1.88 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrädter 1999)
1.93 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log BCF:

1.18 (fathead minnows, Veith et al. 1979b)
0.06 (calculated-\( K_{OW} \), Veith et al. 1980)
1.38; 1.42 (alga \textit{Chlorella fusca}, wet wt. basis; calculated-\( K_{OW} \), Geyer et al. 1984)
0.78 (\textit{P. reticulata}, Canton et al. 1985; quoted, Howard 1989)
1.47 ± 0.12 (guppy-fat wt. basis, Deneer et al. 1987)

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

1.94 (20°C, sorption isotherm-GC, converted from \( K_{OM} \) multiplied by 1.724, Briggs 1981)
2.30 (Lincoln fine sand, calculated explt. value, Wilson et al. 1981)
2.23, 2.57 (Danish subsoils, Loekke 1985)
1.63, 1.84 (two Norwegian organic soils, Seip et al. 1986)
1.70 (soil, quoted, Sabljic 1987)
1.95 ± 0.84, 2.02 ± 1.18; 1.99 (Captina slit loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
1.43 (predicted-\( K_{OW} \), Walton et al. 1992)
1.51 (calculated-\( K_{OW} \), Kollig 1993)
2.20 (soil, calculated-QSAR MCI '\( \chi \)', Sabljic et al. 1995)
2.05, 2.16, 2.15 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)
1.99, 1.84 (RP-HPLC-k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.20; 2.28 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.51, 2.03, 2.26, 2.09, 1.90 (soil: calculated-\( K_{OW} \); HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volutilization: \( t_{1/2}(\text{calc}) = 200 \text{ h} \) from water bodies (Mackay & Leinonen 1975; quoted, Callahan et al. 1979)
\( t_{1/2} = 45 \text{ d} \) was estimated in a model river 1 m deep with a 1.0 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

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Photolysis: aqueous photolysis $t_{1/2} = 67–200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; Howard 1989; Howard et al. 1991); atmospheric photolysis $t_{1/2} = 67–200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; quoted, Howard 1989; Howard et al. 1991); rate constant $k = 2.37 \times 10^{-3}$ 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).

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:

- Phototransformation decay rate constant of 0.17 min$^{-1}$ on 0.20 g/L of TiO$_2$, 8.8 min$^{-1}$ on 0.20 g/L of ZnO and 3.1 min$^{-1}$ on 1.0 g/L of Al$_2$O$_3$ (Minero et al. 1994)

- Abiotic Transformation: Degradation in reductive environment:
  - $k = 0.187$ min$^{-1}$ with solute concn of 50 µM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)
  - $k = (0.16 – < 0.90) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (review, Atkinson 1989)

- Abiotic Transformation: degradation by a soil microflora in more than 64 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)
  - $t_{1/2}(aq. anaerobic) = 48–300$ h, based on anaerobic natural die-away test data for 2,4-dinitrotoluene (Spanggord et al. 1980; quoted, Howard et al. 1991)
  - $k = 14$ mg COD g$^{-1}$ h$^{-1}$ average biodegradation rate for 98% removal (Scow 1982)

- Biodegradation:
  - decomposition by a soil microflora in more than 64 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)
  - $k = (7.39 \pm 1.28) \times 10^{-2}$ M$^{-1}$ s$^{-1}$ in H$_2$S with (mercapto)juglone (an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

- Biotransformation: first-order rate constant of 0.7 d$^{-1}$ corresponding to a half-life of 1 d in adopted activated sludge under aerobic conditions (Mills et al. 1982); rate constant for bacterial transformation of $3 \times 10^{-9}$ mL cell$^{-1}$ h$^{-1}$ in water (Mabey et al. 1982).

Half-Lives in the Environment:
Air: atmospheric lifetimes; $\tau = 180$ d in clean troposphere and $\tau = 90$ d in moderately polluted atmosphere, based on gas-phase reaction with OH radical in atmosphere at room temp. and atmospheric lifetimes $\tau > 6$ yr in clean troposphere and $\tau > 2$ yr in moderately polluted atmosphere, based on gas-phase reaction with O$_3$ (estimated rate constant) in atmosphere at room temp. (Atkinson et al. 1987);
photooxidation $t_{1/2} = 0.544 \text{ to } 5.44 \text{ h}$, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson et al. 1987; quoted, Howard 1989; Howard et al. 1991); atmospheric transformation lifetime was estimated to be $> 5 \text{ d}$ (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 125 \text{ d} \text{ to } 22 \text{ yr}$, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991); estimated $t_{1/2} = 0.3 \text{ to } 3.0 \text{ d}$ in rivers (Zoeteman et al. 1980);

$\text{t}_{1/2} = 322 \text{ to } 4728 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) $t_{1/2}(\text{aerobic}) = 13 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2 \text{ d}$ in natural waters (Capel & Larson 1995).

Groundwater: estimated $t_{1/2} = 1.0 \text{ d}$ in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) $t_{1/2} = 48 \text{ to } 9456 \text{ h}$, based on estimated unacclimated aqueous anaerobic biodegradation half-life for 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated degradation $t_{1/2} = 625 \text{ d}$ in activated sludge (Freitag et al. 1985; quoted, Anderson et al. 1991) $t_{1/2} = 322 \text{ to } 4728 \text{ h}$, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

calculated $t_{1/2} = 9.1 \text{ d}$ from first-order kinetic of degradation rate in sterilized soils (Anderson et al. 1991).

Biota:

**TABLE 16.1.4.1.1**

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<th>Reported aqueous solubilities of nitrobenzene at various temperatures</th>
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<td><strong>Gross et al. 1931</strong></td>
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<td>shake flask-interferometry</td>
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| titration | $\Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = 5.4 \pm 0.2$ at 25°C. |
| 30 | 2060 |
| 50 | 2640 |

**FIGURE 16.1.4.1.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for nitrobenzene.
### TABLE 16.1.4.1.2
Reported vapor pressures of nitrobenzene at various temperatures and the coefficients for the vapor pressure equations

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

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<th>Pressure (Pa)</th>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
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*complete list see ref.
FIGURE 16.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for nitrobenzene.
16.1.4.2 2-Nitrotoluene

Common Name: 2-Nitrotoluene
Synonym: 1-methyl-2-nitrobenzene, o-nitrotoluene, 2-methylnitrobenzene
Chemical Name: 2-nitrotoluene, o-nitrotoluene
CAS Registry No: 88-72-2
Molecular Formula: C₇H₇NO₂, CH₃C₆H₄NO₂
Molecular Weight: 137.137
Melting Point (°C):
-10.4 (Lide 2003)
Boiling Point (°C):
222 (Lide 2003)
Density (g/cm³ at 20°C):
1.15693, 1.15232 (20°C, 25°C, Dreisbach & Martin 1949)
1.1629 (Weast 1982–83)
Molar Volume (cm³/mol):
117.9 (20°C, Stephenson & Malanowski 1987)
153.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 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):
652 (30°C, shake flask-interferometer, Gross et al. 1933)
656 (quoted, Deno & Berkheimer 1960)
< 233 (shake flask-centrifuge, Booth & Everson 1948)
324 (Hansch et al. 1968)
656, 2076 (quoted, predicted-KₒₐW, Valvani et al. 1981)
652 (30°C, Verschueren 1983)
656, 771 (quoted, calculated-fragment const., Wakita et al. 1986)
641: 444 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
609* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)
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):
23.97* (extrapolated-regression of tabulated data, Kahlbaum 1898)
27.69* (extrapolated-regression of tabulated data, temp range 50–222.3°C, Stull 1947)
log (P/mmHg) = 7.49454 – 2086.1/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
log (P/mmHg) = [–0.2185 × 12239.7/(T/K)] + 8.286642; temp range 50–222.3°C (Antoine eq., Weast 1972–73)
13.33 (20°C, Verschueren 1983)
1.670 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.01415 – 967.744/(99.208 + t°C); temp range 129.31–222.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.440 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 5.851 – 946/(96 + t°C), temp range 129–222°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 6.32043 – 1827.66/(–71.63 + T/K); temp range 402–496 K (Antoine eq., Stephenson & Malanowski 1987)
24.80° (ebulliometry, average from extrapolated-Antoine eq., Aim 1994)

\[
\log (P/\text{mmHg}) = 7.8266 - 2.9906 \times 10^3/(T/K) + 1.1064 \log (T/K) + 2.2375 \times 10^{-6}(T/K)^2;
\]

temp range 270–720 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
5.811 (exptl., Hine & Mookerjee 1975)
4.723, 4.616 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
2.30 (Leo et al. 1971; Hansch & Leo 1985)
2.30 (HPLC-k correlation, Deneer et al. 1987)
2.30 (unpublished data quoted from CLOGP Database and recommended, Sangster 1989)
2.39, 2.43, 2.58 (CPC-RV correlation, Gluck & Martin 1990)
2.46, 2.60; 2.30 (25°C, 60°C, shake flask-UV; quoted lit. value, Kramer & Henze 1990)
2.13 (shake flask-UV, Nakagawa et al. 1992)
2.30 (recommended, Sangster 1993)
2.40 ± 0.15, 2.21 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):
< 2.0 (carprinus carpio, Sasaki 1978; Kawasaki 1980)
1.52, 1.20 (calculated-\( K_{OW} \), S, Lyman et al. 1982; quoted, Howard 1989)
2.28 ± 0.06 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log \( K_{OC} \):
2.63, 2.09 (soil, calculated-\( K_{OW} \), S, Lyman et al. 1982; quoted, Howard 1989)

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

Volutilization: estimated \( t_{1/2} = 21 \) h using Henry’s law constant for a model river 1-m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:
Oxidation: rate constant \( k = 3.0 \times 10^{-11} \) cm³ molecules⁻¹ s⁻¹ for the reaction with \( 8 \times 10^{-5} \) molecules/cm³ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); rate constant \( k = 7.0 \times 10^{-11} \) cm³ molecule⁻¹ s⁻¹ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989).

Hydrolysis:
Abiotic Transformation: Degradation in reductive environment:
\( k = 0.141 \) min⁻¹ with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

Biodegradation: average biodegradation rate of 32.5 mg COD g⁻¹ h⁻¹ for 98% removal (Scow 1982).
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Air: \( t_{1/2} = 8 \) h, based on a rate constant \( k = 3.0 \times 10^{-11} \) cm³ molecules⁻¹ s⁻¹ for the reaction with \( 8 \times 10^{-5} \) molecules/cm³ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989).
Surface water: estimated \( t_{1/2} = 3.2 \) d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
midday \( t_{1/2}(\text{calc}) = 45 \) min in Aucilla River water due to indirect photolysis using an experimentally determined reaction rate constant \( k = 0.92 \) h⁻¹ (Zepp et al. 1984; quoted, Howard 1989);
estimated \( t_{1/2} = 3.2 \) d for a river 4 to 5 m deep, based on monitoring data (Zoeteman et al. 1980; quoted, Howard 1989).

Ground water:
Sediment:
Soil:
Biota:
TABLE 16.1.4.2.1  
Reported aqueous solubilities of 2-nitrotoluene at various temperatures

<table>
<thead>
<tr>
<th>Gross et al. 1931</th>
<th>Beneš &amp; Dohnal 1999</th>
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<tbody>
<tr>
<td>shake flask-interferometry</td>
<td>shake flask-UV</td>
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<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
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<tr>
<td>15</td>
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<td>30</td>
<td>652</td>
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<td>30</td>
<td>688</td>
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<tr>
<td>40</td>
<td>773</td>
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</table>

ΔHsol/(kJ mol⁻¹) = 9.4 ± 0.1

25°C

FIGURE 16.1.4.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-nitrotoluene.

TABLE 16.1.4.2.2  
Reported vapor pressures of 2-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Kahlbaum 1898 static method</th>
<th>Stull 1947 summary of literature data</th>
<th>Dreisbach &amp; Shrader 1949 ebulliometry</th>
<th>Aim 1994 comparative ebulliometry</th>
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</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
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<td>81.8</td>
<td>666.6</td>
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<td>94.8</td>
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<td>79.1</td>
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<td>109.6</td>
<td>2666.4</td>
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<tr>
<td>114.8</td>
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**TABLE 16.1.4.2.2 (Continued)**

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<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Aim 1994</th>
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<td>static method</td>
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<td>ebulliometry</td>
<td>comparative ebulliometry</td>
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<td>185.48</td>
<td>42077</td>
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<td>13332</td>
<td>205.48</td>
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<td>197.7</td>
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<td>186.1</td>
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</tr>
<tr>
<td>172.4</td>
<td>26664</td>
<td>222.3</td>
<td>101325</td>
<td>bp/°C</td>
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<td>196.0</td>
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</table>

**FIGURE 16.1.4.2.2** Logarithm of vapor pressure versus reciprocal temperature for 2-nitrotoluene.

2-Nitrotoluene: vapor pressure vs. 1/T

- b.p. = 222 °C
- m.p. = -10.4 °C

Kahlbaum 1898
Dreisbach & Shrader 1949
Aim 1994
Stull 1947

mp/°C = –2.90
bp/°C = 222.946

eq. 3
A = 6.45342
B = 1906.532
C = 65.441

For temp range: 115–175°C
16.1.4.3 4-Nitrotoluene

Common Name: 4-Nitrotoluene
Synonym: 1-methyl-4-nitrobenzene, p-nitrotoluene, 4-methylnitrobenzene
Chemical Name: 4-nitrotoluene, p-nitrotoluene
CAS Registry No: 99-99-0
Molecular Formula: CH₃C₆H₄NO₂
Molecular Weight: 137.137
Melting Point (°C):
51.63  (Lide 2003)
Boiling Point (°C):
238.3  (Stull 1947; Weast 1982–83; Dean 1985; Howard 1989)
Density (g/cm³ at 20°C):
1.16278, 1.15799 (20°C, 25°C, Dreisbach & Martin 1949)
1.392  (Dean 1985)
Molar Volume (cm³/mol):
124.2  (75°C, Stephenson & Malanowski 1987)
153.0  (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
–11.27  (Perrin 1972)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
17.15  (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_fus (J/mol K):
50.21  (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.548 (mp at 51.63°C)

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):
442  (30°C, shake flask-interferometer, Gross et al. 1933)
< 278  (shake flask-centrifuge, Booth & Everson 1948)
302  (Tsonopoulos & Prausnitz 1971)
442  (30°C, Verschueren 1983)
288  (20°C, shake flask-UV spectrophotometry, Hashimoto et al. 1984)
307  (calculated-group contribution method, Kühne et al. 1995)
242*  (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 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):
13.98*  (extrapolated-regression of tabulated data, measured range 92–237°C, Kahlbaum 1898)
log (P/mmHg) = –2630/(T/K) + 8.025  (isoteniscopie method, temp range not specified, Kobe et al. 1941)
22.81*  (extrapolated-regression of tabulated data, temp range 53.7–238.2°C, Stull 1947)
log (P/mmHg) = 7.52323 – 2150.6/(230 + t°C)  (Antoine eq., Dreisbach & Martin 1949)
8851*  (147.1°C, ebulliometry, measured range 147.71–233.25°C, Dreisbach & Shrader 1949)
log (P/mmHg) = 11.5424 – 4130.0708/(T/K); temp range 297–310 K  (Knudsen effusion, Lenchitz & Velicky 1970)
log (P/mmHg) = [–0.2185 × 11915.0/(T/K)] + 7.965025; temp range 53.7–238.3°C  (Antoine eq., Weast 1972–73)
5.50*  (ebulliometry, fitted to Antoine eq., measured range 144–239°C, Ambrose & Gundry 1980)
9.50  (extrapolated-supercooled liq., Ambrose & Gundry 1980)
Nitrogen and Sulfur Compounds

8.347 (extrapolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 6.11507 – 1716.897/(184.543 + t°C); temp range 147.7–233.3°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
8.38 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.9948 – 1720.39/(184.9 + t°C); temp range 148–233°C (Antoine eq., Dean 1985, 1992)
0.653 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 10.6673 – 4130.07/(T/K); temp range 296–310 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 7.40605 – 2889.12/(23.37 + T/K); temp range 423–512 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
15.18* (ebulliometry, average of extrapolated-Antoine eq., Aim 1994)
log (P/mmHg) = 9.9641 – 2.6549 × 10³/(T/K) – 0.80182·log (T/K) + 5.3926 × 10–4·(T/K) – 4.109 × 10–14·(T/K)²;
temp range 325–736 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
5.065 (calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log Kₐw:
2.37 (shake flask-UV, Fujita et al. 1964)
2.40 (unpublished result, Leo et al. 1971)
2.34 (HPLC-k' correlation, Deneer et al. 1987)
2.42 (recommended, Sangster 1989)
2.10, 2.05 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
2.61 (shake flask-UV, Nakagawa et al. 1992)
2.37 (recommended, Sangster 1993)
2.37 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
2.42 (recommended, Hansch et al. 1995)
2.18 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log Kₐa:

Bioconcentration Factor, log BCF:
< 2.0 (Carassius carpio, Sasaki 1978; Kawasaki 1980)
1.57, 1.30 (calculated-Kₐw S, Lyman et al. 1982; quoted, Howard 1989)
2.37 ± 0.05 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log Kₐc:
2.67, 2.18 (soil, calculated-Kₐw S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:
Volatilization: based on Henry’s law constant an estimated t₁/₂ = 25 h was obtained for a model river of 1- m deep with a current of 1 m/s and wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: photooxidation t₁/₂ = 8.0 h in air, based on measured rate constant k = 3 × 10−11 cm³ molecule⁻¹ s⁻¹ at 25°C for the reaction with photochemically produced 8 × 10⁵ molecules/cm³ hydroxyl radical (GEMS 1986; quoted, Howard 1989).
Hydrolysis:
Abiotic Transformation: Degradation in reductive environment:
k = 0.101 min⁻¹ with solute concn of 50 µM in a 19 d-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Kluesen et al. 1995)
Biotransformation:
average biodegradation rate of 32.5 mg COD g⁻¹ h⁻¹ for 98% removal (Scow 1982).
Biocatalysis:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
Half-Lives in the Environment:

Air: photooxidation t₁/₂ = 8.0 h, based on measured rate constant of 3 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 25°C for the reaction with photochemically produced 8 × 10⁵ molecules/cm³ hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Surface water: estimated t₁/₂ = 2.7 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) estimated t₁/₂ = 2.7 d, based on monitoring data for a river of 4 to 5-m deep (Zoeteman et al. 1980; quoted, Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

### TABLE 16.1.4.3.1
Reported aqueous solubilities of 4-nitrotoluene at various temperatures

<table>
<thead>
<tr>
<th>Gross et al. 1931</th>
<th>Beneš &amp; Dohnal 1999</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-interferometry</td>
<td>shake flask-UV</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>15</td>
<td>-</td>
</tr>
<tr>
<td>30</td>
<td>442</td>
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<td>30</td>
<td>322</td>
</tr>
<tr>
<td>40</td>
<td>418</td>
</tr>
</tbody>
</table>

ΔHₘₚ/(kJ mol⁻¹) = 21.1 ± 0.1

25°C

![Figure 16.1.4.3.1](image)

**FIGURE 16.1.4.3.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-nitrotoluene.
TABLE 16.1.4.3.2
Reported vapor pressures of 4-nitrotoluene 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.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
<th>Log P</th>
<th>ln P</th>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
<th>Log P</th>
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<td>92.3</td>
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<td>at 298.15 K P = 5.5Pa</td>
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#### FIGURE 16.1.4.3.2

Logarithm of vapor pressure versus reciprocal temperature for 4-nitrotoluene.
16.1.4.4 2,4-Dinitrotoluene (DNT)

Common Name: 2,4-Dinitrotoluene
Synonym: dinitrotoluol, 1-methyl-2,4-dinitrobenzene, DNT
Chemical Name: 2,4-dinitrotoluene, 1-methyl-2,4-dinitrobenzene
CAS Registry No: 121-14-2
Molecular Formula: C₇H₆N₂O₄, CH₃C₆H₃(NO₂)₂
Molecular Weight: 182.134
Melting Point (°C):
70.5 (Lide 2003)
Boiling Point (°C):
300 dec. (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
1.521 (15°C, Verschueren 1983)
Molar Volume (cm³/mol):
175.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
-13.53 (Perrin 1972)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
58.99 (Yalkowsky & Valvani 1980)
Entropy of Fusion, ΔS_fus (J/mol K):
58.99 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.358 (mp at 70.5°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):
270 (22°C, Verschueren 1977, 1983)
300 (22°C, Dunlap 1981)
276; 145 (quoted expitl.; calculated-group contribution method, Kühne et al. 1995)
199 (25.2°C, shake flask-HPLC/UV, Phelan & Barnett 2001)
188* (22°C, shake flask-HPLC/UV, measured range 12.4–61.8°C, Phelan & Barnett 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):
0.133* (59°C, Knudsen effusion, measured range 59–69°C, Lenchitz & Velicky 1970)
0.00321 (extrapolated-Antoine eq., Lenchitz & Velicky 1970)
log (P/mmHg) = 12.6177 – 5139.058/(T/K); temp range 331.913–342.277 K (Knudsen effusion, Lenchitz & Velicky 1970)
0.0177* (20°C, gas saturation-GC/ECD, measured range 277.5–344.15 K, Pella 1977)
0.0290 (gas saturation-GC/ECD, interpolated-Antoine eq., measured range 277.5–344.15 K Pella 1977)
log (P/kPa) = 5.06336 – 1216.523/(76.54 + t°C); temp range 100–199°C (Antoine eq. from reported expitl. data, Boublik et al. 1984)
0.0296, 0.0032 (extrapolated-Antoine eq.-I, eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 12.27361 – 5009.432/(T/K); temp range 277–343 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 11.7426 – 5139.058/(T/K); temp range 331–342 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/Pa) = 7.1423 - 3039/(T/K); temp range 473–572 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/Pa) = 6.04898 - 1956.095/(-108.183 + T/K); temp range 344–572 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/mmHg) = 5.798 - 1118/(61.8 + t/°C); temp range 200–299°C (Antoine eq., Dean 1992)
log (P/mmHg) = 11.5966 - 3.0079 × 10³/(T/K) -1.6468·log (T/K) + 1.5949 × 10⁻³·(T/K) - 1.8722 × 10⁻¹⁴·(T/K)²; temp range 343–814 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.0160 (calculated-P/C, Smith et al. 1981)
- 0.4560 (calculated-P/C, Mabey et al. 1982)
- 0.0878 (Smith et al. 1983; quoted, Howard 1989)
- 32.23 (quoted from WERL Treatability database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K OW:
- 1.98 (shake flask, Hansch & Leo 1985)
- 2.04 (HPLC-k′ correlation, Den eer et al. 1987)
- 1.98 (recommended, Sangster 1993)
- 1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K OA:

Bioconcentration Factor, log BCF:
- 1.59 (microorganisms-water, calculated-K OW, Mabey et al. 1982)
- 1.11, 1.76 (daphnia magna, lumbriculus variegatus, Liu et al. 1983)
- > 3.30 (selanastrum capricornutum, Liu et al. 1983)
- 1.89, 0.602 (bluegill sunfish in viscera, bluegill sunfish in muscle, Liu et al. 1983)
- 2.31 ± 0.03 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K OC:
- 1.65 (sediment-water, calculated-K OW, Mabey et al. 1982)
- 1.68 (calculated-K OW, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t ½:
Volatilization: half-life of approximately 100 d (Mills et al. 1982).
Photolysis: direct photolysis rate constant k = 1.6 × 10⁻² h⁻¹ for summer at 40°N latitude in water (Mabey et al. 1982);
aqueous photolysis t ½ = 23–72 h, based on measured photolysis rates in water (Mill & Mabey 1985; Simmons & Zepp 1986; quoted, Howard et al. 1991);
atmospheric transformation lifetime τ ~ 1–5 d (Kelly et al. 1994).
Hydrolysis:
Oxidation: aqueous oxidation rate constants k << 360 M⁻¹ h⁻¹ for singlet oxygen and k = 144 M⁻¹ h⁻¹ for peroxy radical at 25°C (Mabey et al. 1982);
photooxidation t ½ = 284 – 2840 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
photooxidation t ½ = 3–33 h, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991).
Biodegradation: aqueous anaerobic t ½ = 48–240 h, based on anaerobic natural water die-away test data (Spanggord et al. 1980; quoted, Howard et al. 1991); aqueous aerobic t ½ = 672–4320 h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).
Biotransformation: rate constant of 1 × 10⁻² mL cell⁻¹ h⁻¹ for bacterial transformation in water (Mabey et al. 1982).
Bioconcentration, Uptake (k ½) and Elimination (k ½) Rate Constants:
Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 284–2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime $\tau \sim 1–5$ d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 3–33$ h, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991);
estimated $t_{1/2} = 1.7$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
sunlight photolysis $t_{1/2} \sim 42$ h in pure water but ranged from 3 h to 10 h in three natural waters (Mabey et al. 1982).

Groundwater: $t_{1/2} = 48 – 8640$ h, based on estimated unacclimated aqueous anaerobic and 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:

**TABLE 16.1.4.4.1**

Reported aqueous solubilities and vapor pressures of 2,4-dinitrotoluene at various temperatures and the coefficients for the vapor pressure equations

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<th>Aqueous solubility</th>
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</tbody>
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enthalpy of sublimation:
\[ \Delta H_{\text{subl}} = 98.324 \text{ kJ mol}^{-1} \] (at 25°C)

enthalpy of sublimation:
\[ \Delta H_{\text{subl}} = 95.81 \text{ kJ mol}^{-1} \]
FIGURE 16.1.4.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dinitrotoluene.
16.1.4.5 2,6-Dinitrotoluene

Common Name: 2,6-Dinitrotoluene
Synonym: dinitrotoluel, 1-methyl-2,6-dinitrobenzene, 2-methyl-1,3-dinitrobenzene
Chemical Name: 2,6-dinitrotoluene, 1-methyl-2,6-dinitrobenzene
CAS Registry No: 606-20-2
Molecular Formula: C7H6N2O4, CH3C6H3(NO2)2
Molecular Weight: 182.134
Melting Point (°C):
   66.0 (Weast 1982–83; Howard 1989; Lide 2003)
Boiling Point (°C):
   285 (Verschueren 1977; Callahan et al. 1979; Howard 1989; Lide 2003)
Density (g/cm³ at 20°C):
   1.2833 (111°C, Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
   141.9 (111°C, Stephenson & Malanowski 1987)
   175.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 0.396 (mp at 66.0°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated.):
   180 (20°C, estimated, Mabey et al. 1982)
   300 (selected, Mills et al. 1982)
   182; 155 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
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):
   0.0756* (gas saturation-GC/ECD, fitted to Antoine eq., temp range 277.5–323.15 K, Pella 1977)
   log (P/mmHg) = (13.99 ± 0.18) – (5139 ± 52)/(T/K), temp range 277.5–323.15 K (gas saturation, Pella 1977)
   0.0756 (Howard et al. 1986; quoted, Banerjee et al. 1990)
   0.0767 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P/kPa) = 11.9436 – 4446.22/(–21.279 + T/K); temp range 277–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P/kPa) = 7.329 – 2971/(T/K); temp range 423–523 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
   log (P/kPa) = 6.70024 – 2160.968/(–93.282 + T/K); temp range 330–770 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C)
   0.800 (calculated-P/C, Mabey et al. 1982)
   32.23 (quoted from WERL Treatability database, Ryan et al. 1988)
   0.022 (SOGC 1987; quoted, Howard 1989)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 1.72 (shake flask, Hansch & Leo 1985)
- 2.02 (HPLC-k correlation, Deneer et al. 1987)
- 2.02 (shake flask-HPLC, Leggett et al. 1992)
- 2.07 (shake flask-UV, Nakagawa et al. 1992)
- 2.06 (recommended, Sangster 1993)
- 2.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- 3.72 (algal biomass, Davis et al. 1981)
- 1.71 (microorganisms-water, calculated-K$_{OW}$, Mabey et al. 1982)
- 1.08 (calculated-K$_{OW}$, Lyman et al. 1982; quoted, Howard 1989)
- 2.44 ± 0.04 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log $K_{OC}$:
- 1.96 (sediment-water, calculated-K$_{OW}$, Mabey et al. 1982)
- 2.31 (soil, calculated-K$_{OW}$, Lyman et al. 1982; quoted, Howard 1989)
- 1.40 (calculated-K$_{OW}$, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- Volatilization: $t_{1/2} \sim 100$ d (Mills et al. 1982).
  89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).
- Hydrolysis:
  - Oxidation: aqueous oxidation rate constants $k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 144$ M$^{-1}$ h$^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
  - photooxidation $t_{1/2} = 2–17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991);
  - photooxidation $t_{1/2} = 284–2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- Biodegradation: aqueous anaerobic $t_{1/2} = 48–300$ h, based on anaerobic natural water die-away test data for 2,4-dinitrotoluene; aqueous aerobic $t_{1/2} = 672–4320$ h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).
- Biotransformation: $k = 1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacterial transformation in water (Mabey et al. 1982)
- Biotransformation in marine sediments: all broken down in 28 d when incubated at 10°C, and in 7 d when incubated at 20°C in the sandy sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grained sediment (Nipper et al. 2004).

Bioconcentration, Uptake ($k_{1}$) and Elimination ($k_{2}$) Rate Constants:

Half-Lives in the Environment:
- Air: estimated atmospheric $t_{1/2} = 8$ h, based on the vapor phase reaction with hydroxyl radical in air (GEMS 1985; quoted, Howard 1989); photolysis $t_{1/2} = 284–2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- Surface water: midday $t_{1/2} \sim 12$ min in Aucilla river due to indirect photolysis using experimentally determined rate constant $k = 3.6$ h$^{-1}$ (Zepp et al. 1984);
  - photolysis $t_{1/2} = 2–17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991);
  - 89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).
- Ground water: $t_{1/2} = 48–8640$ h, based on estimated unacclimated aqueous anaerobic biodegradation half-life 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: degraded by days 28 and 7 for incubation at 10 and 20°C, respectively, in sandy marine sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grain sediment (Nipper et al. 2004)

Soil: $t_{1/2} = 672 - 4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

### TABLE 16.1.4.5.1

Reported vapor pressures of 2,6-dinitrotoluene at various temperatures

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<tr>
<td>10.0</td>
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<td>0.483</td>
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<tr>
<td>eq. 1</td>
<td>P/mmHg</td>
</tr>
<tr>
<td>( \log P = A - B/(T/K) )</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>13.99</td>
</tr>
<tr>
<td>B</td>
<td>5139</td>
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</tbody>
</table>

enthalpy of sublimation:

\[ \Delta H_{subl} = 98.324 \text{ kJ mol}^{-1} \]

### FIGURE 16.1.4.5.1

2,6-Dinitrotoluene: vapor pressure vs. $1/T$

**FIGURE 16.1.4.5.1** Logarithm of vapor pressure versus reciprocal temperature for 2,6-dinitrotoluene.
16.1.4.6 2,4,6-Trinitrotoluene (TNT)

Common Name: 2,4,6-Trinitrotoluene
Synonym: TNT
Chemical Name: 2,4,6-trinitrotoluene
CAS Registry No: 118-96-7
Molecular Formula: C₇H₅N₃O₆, (NO₂)₃C₆H₂CH₃
Molecular Weight: 227.131
Melting Point (°C):
80.5 (Lide 2003)
Boiling Point (°C):
240 explodes (Weast 1982–83; Dean 1992; Lide 2003)
Density (g/cm³):
1.654 (20°C, Weast 1982–83; Dean 1992)
Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
137.3 (20°C, calculated-density)
187.1 (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: 0.285 (mp at 80.5°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):
120* (20°C, shake flask, measured range 0.30–99.5°C, Taylor & Rinkenbach 1923)
85.8 (21°C, Hale et al. 1979)
200 (15°C, Verschueren 1983)
100 (Dean 1992)
101.5* (average value at pH < 9.1, shake flask-HPLC/UV, measured range 6–42°C, Ro et al. 1996)
101.6, 100.5, 110.5 (pH 4.2, 5.7, 6.2, shake flask-HPLC/UV, measured range 2.3–38°C, Lynch 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):
0.352* (53°C, Knudsen effusion, measured range 50–143°C, Edwards 1950)
log (P/cmHg) = 14.34 – 6180/(T/K); range 50–81°C (solid, Knudsen effusion, Edwards 1950)
log (P/cmHg) = 10.90 – 4960/(T/K); range 81–143°C (liquid, Knudsen effusion, Edwards 1950)
0.0568* (54.76°C, Knudsen effusion, measured range 55–76°C, Lenchitz & Velicky 1970)
log (P/mmHg) = 13.0776 – 5400.536/(T/K); temp range 55–76°C (Knudsen effusion, Lenchitz & Velicky 1970)
0.00107* (gas saturation-GC/ECD, measured range 287.15–329.65 K, Pella 1977)
log (P/mmHg) = (12.31 ± 0.34) – (5175 ± 105)/(T/K); temp range 287.15–329.65 K (gas saturation, Pella 1977)
log (P/kPa) = 7.36331 – 3199.923/(248.004 + t°C); temp range 230–250°C (liquid, Antoine eq. from reported
eq exp. data, Boublík et al. 1984)
0.00078 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\[
\log (P_s/kPa) = 13.596 - 5874.238/(T/K); \text{ temp range 293–353 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P_s/kPa) = 12.2025 - 5400.536/(T/K); \text{ temp range 337–350 K (solid, Antoine eq.-II., Stephenson & Malanowski 1987)}
\]
\[
\log (P_L/kPa) = 6.40336 - 2191.85/(-121.43 + T/K); \text{ temp range 353–523 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P/mmHg) = 7.67152 - 2669.4/(205.6 + t/°C); \text{ temp range 230–250°C (Antoine eq., Dean 1992)}
\]
\[
\log (P/mmHg) = 6.3156 - 2.6756 \times 10^3/(T/K) - 4.6215 \times 10^{-9} \times (T/K) - 2.3743 \times 10^{-12} \times (T/K)^2; \text{ temp range 354–518 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, \(K_{OW}\):
- 1.60 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.8 (shake flask-HPLC, Leggett et al. 1992)
- 1.73 (recommended, Sangster 1993)
- 2.05 (estimated-SPARC, Elovitz & Weber 1999)

Octanol/Air Partition Coefficient, \(K_{OA}\):

Bioconcentration Factor, \(log \text{BCF or } K_O\):
- 1.09 (aquatic oligochaete \text{Tubifex tubifex}, Conder et al. 2004)

Sorption Partition Coefficient, \(K_{SC}\):

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

Volatilization:

\text{Photolysis: } t_{1/2} = 14 \text{ h in summer}, t_{1/2} = 22–84 \text{ h in winter in pure water and photolyzed very rapidly in natural waters (Mabey et al. 1983)}

\text{photocatalytic degradation rates of TNT in a circular photocatalytic reactor using a UV lamp as a light source and TiO}_2 \text{ as a photocatalyst: } 1) \text{ at different initial TNT concns: } \text{k = 0.0989 min}^{-1} \text{ with } t_{1/2} = 7.07 \text{ min at initial concn of 10 mg/L; k = 0.0644 min}^{-1} \text{ with } t_{1/2} = 10.76 \text{ min at initial concn of 20 mg/L; k = 0.0405 min}^{-1} \text{ with } t_{1/2} = 17.11 \text{ min at initial concn of 30 mg/L; k = 0.0269 min}^{-1} \text{ with } t_{1/2} = 25.77 \text{ min at initial concn of 50 mg/L; and k = 0.0165 min}^{-1} \text{ with } t_{1/2} = 42.01 \text{ min at initial concn of 100 mg/L. 2) at different pH: k = 0.0173 min}^{-1} \text{ with } t_{1/2} = 27.6 \text{ min at pH 3.0; k = 0.0422 min}^{-1} \text{ with } t_{1/2} = 20.1 \text{ min at pH 7.0 and k = 0.0451 min}^{-1} \text{ with } t_{1/2} = 21.5 \text{ min at pH 11.0 (Son et al. 2004)}}

\text{Photooxidation: }

\text{Hydrolysis: }

\text{Biodegradation: 95\% disappearance within 2 h under aerobic conditions, and complete loss within 10 min under anaerobic conditions in sediment-water systems (Elovitz & Weber 1999)}

\text{Biotransformation: 100\% biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)}

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

Half-Lives in the Environment:

\text{Air: }

\text{Surface water: photolysis } t_{1/2} = 14 \text{ h in summer}, t_{1/2} = 22–84 \text{ h in water in pure water, less than 1/2 h in some natural waters (Mabey et al. 1983)}

\text{photocatalytic degradation } t_{1/2} = 7.07 \text{ min to 42.1 min for different initial concn of TNT from 10- 100 mg/L, and } t_{1/2} = 27.1 – 21.5 \text{ min at pH 3.0–7. 0 in a circular reactor, using a UV lamp as a light source and TiO}_2 \text{ as a photocatalyst (Son et al. 2004)}

\text{Ground water: }

\text{Sediment: rapid disappearance 95\% within 2 h, of TNT in an aerobic sediment-water system; under anaerobic conditions, TNT loss was complete within 10 min (Elovitz & Weber 1999)}
100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

Soil:
Biota: steady-state concn reached within 1-h in uptake experiments, and TNT depuration after a 24-h exposure occurred completely by 3 h (aquatic oligochaete, Conder et al. 2004)

<table>
<thead>
<tr>
<th>TABLE 16.1.4.6.1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reported aqueous solubilities of 2,4,6-trinitrotoluene (TNT) at various temperatures</strong></td>
</tr>
</tbody>
</table>

\[
\ln S = A - B/(T/K) \quad (1)
\]

1.

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<tbody>
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<td>shake flask-HPLC/UV</td>
<td>shake flask-HPLC/UV</td>
<td>shake flask-HPLC/UV</td>
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<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>
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<td>0.30</td>
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<td>average of 3 sets of data</td>
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</tr>
</tbody>
</table>

\[
\ln [S/(\text{mg/L})] = 16.12 - 3413/(T/K)
\]
for \( \text{pH} < 8 \)

2.

<table>
<thead>
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<th>lynch et al. 2001</th>
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</thead>
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<tr>
<td>shake flask-HPLC/UV</td>
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<td>( t/°C )</td>
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<tr>
<td>pH 4.2</td>
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<tr>
<td>pH 5.7</td>
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<td>pH 6.2</td>
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TABLE 16.1.4.6.1 (Continued)

Lynch et al. 2001

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<th>t/°C</th>
<th>S/g·m⁻³</th>
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<td>100.6</td>
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<td>99.5</td>
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<tr>
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<td>97.5</td>
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<tr>
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<td>97.8</td>
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<td>100.4</td>
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<td>97.2</td>
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<td>211.7</td>
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<td>36</td>
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<td>37.7</td>
<td>228.3</td>
<td>38</td>
<td>235</td>
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</table>

eq. 1 S/(mg L⁻¹) eq. 1 S/(mg L⁻¹) eq. 1 S/(mg L⁻¹)

A 22.741 A 22.399 A 23.244
B 6332 B 6230 B 6506.8

composite correlation eq.: \( \ln \left[ \frac{S}{(\text{mg L}^{-1})} \right] = 16981 - \frac{3607.5}{(T/\text{K})} \); temp range 2.3–38°C

FIGURE 16.1.4.6.1 Logarithm of mole fraction solubility (ln \( x \)) versus reciprocal temperature for 2,4,6-trinitrotoluene.
**TABLE 16.1.4.6.2**  
Reported vapor pressures of 2,4,6-trinitrotoluene (2,4,6-TNT) at various temperatures and the coefficients for the vapor pressure equations

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

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</tr>
</thead>
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<tr>
<td></td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>Knudsen method</td>
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<td>25.0</td>
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<tr>
<td>82.4</td>
<td>1.0612</td>
<td>mp/°C</td>
<td>81.1</td>
</tr>
<tr>
<td>86.9</td>
<td>1.5865</td>
<td></td>
<td></td>
</tr>
<tr>
<td>99.5</td>
<td>5.2529</td>
<td>enthalpy of sublimation:</td>
<td></td>
</tr>
<tr>
<td>99.5</td>
<td>5.4262</td>
<td>ΔH&lt;sub&gt;subl&lt;/sub&gt; = 120.92 kJ mol&lt;sup&gt;-1&lt;/sup&gt; (at 25°C)</td>
<td>eq. 2</td>
</tr>
<tr>
<td>110.6</td>
<td>11.012</td>
<td></td>
<td>A</td>
</tr>
<tr>
<td>110.5</td>
<td>10.612</td>
<td></td>
<td>B</td>
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<td>131.5</td>
<td>46.396</td>
<td>enthalpy of sublimation:</td>
<td></td>
</tr>
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<td>141.4</td>
<td>82.793</td>
<td>eq. 1 P/mmHg</td>
<td>A</td>
</tr>
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<td>142.0</td>
<td>87.728</td>
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<td>5400.536</td>
</tr>
<tr>
<td>142.5</td>
<td>82.260</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For solid:
- eq. 1 P/cmHg
  - A 14.34
  - B 6180

ΔH<sub>subl</sub> = 118.41 kJ mol<sup>-1</sup>

For liquid:
- eq. 1 P/cmHg
  - A 10.90
  - B 4960

ΔH<sub>subl</sub> = 94.98.34 kJ mol<sup>-1</sup>
FIGURE 16.1.4.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trinitrotoluene.
16.1.4.7 1-Nitronaphthalene (α-Nitronaphthalene)

Common Name: 1-Nitronaphthalene
Synonym: α-nitronaphthalene
Chemical Name: 1-nitronaphthalene, α-nitronaphthalene
CAS Registry No: 86-57-7
Molecular Formula: C_{10}H_{7}NO_{2}
Molecular Weight: 173.169
Melting Point (°C):
61 (Lide 2003)
Boiling Point (°C):
304.0 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987)
Density (g/cm³ at 20°C):
1.3320 (Weast 1982–83)
1.2230 (Dean 1985)
Molar Volume (cm³/mol):
176.1 (calculated-Le Bas method at normal boiling point)
135.8 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.99 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.39 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.443 (mp at 61°C)
Water Solubility (g/m³ or mg/L at 25°C):
50.0 (Aqueous Solubility Database, Yalkowsky et al. 1987)
9.82 (generator column-HPLC/UV, Yu & Xu 1992)
9.83 (calculated-molar concentration, Yu & Xu 1992)
50; 34.6 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.202 (effusion method-fitted to Antoine eq., Radchenko & Kitiagorodskii 1974)
0.202 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
0.184 (liquid, extrapolated-Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_s/kPa) = 8.31261 – 3579.698/(T/K); temp range 309–326 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 13.223 – 5584/(T/K); temp range 325–332 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_s/kPa) = 7.8959 – 3468.4/(T/K); temp range 332–580 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
3.463 (calculated-P/C with selected values)
0.178 (gas stripping-GC, Altschuh et al. 1999)
Octanol/Water Partition Coefficient, log K_{ow}:
3.19 (Hansch & Leo 1979)
3.19 (shake flask, Hansch & Leo 1987)
Nitrogen and Sulfur Compounds

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, $t_\text{½}$:

- **Volatilization:**
  - Photolysis: measured photolysis rate constant are: $15.9 \times 10^{-4}$ s$^{-1}$ in a 6400-L indoor all-Teflon chamber under blacklamp irradiation and $1.37 \times 10^{-4}$ s$^{-1}$ outdoor in a 1000-L all-Teflon chamber under natural solar irradiation (Atkinson et al. 1989);
  - Photolysis rate $k_{\text{phot}} = 1.5 \times 10^{-4}$ s$^{-1}$ with a half-life of 1.7 h (Arey et al. 1990)

- **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:
    - $k_{OH} = (5.4 \pm 1.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{NO3} \leq 7.2 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O3} < 6.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{N2O5} = 1.3 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with N$_2$O$_5$ and at 298 ± 2 K in the atmosphere (Atkinson et al. 1989)
    - $k_{OH} = 5.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated lifetime of 2.9 d; $k_{NO3} \leq 7.2 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with calculated lifetime of ~13 d, $k_{O3} < 6.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a lifetime of > 28 d and $k_{N2O5} = 1.3 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with N$_2$O$_5$ a calculated lifetime of 2.4 yr at 298 ± 2 K in the atmosphere (Arey et al. 1990)

- **Biodegradation:**
- **Biotransformation:**
- **Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**

Half-Lives in the Environment:

- **Air:** calculated lifetime of ~2 h based on measured outdoor photolysis rate and rate constants the gas-phase reactions (Atkinson et al. 1989);
  - Photolysis $t_\text{½} = 1.7$ h using an average 12-h daytime NO$_2$ photolysis rate $k = 5.2 \times 10^{-3}$ s$^{-1}$ – a dominant atmospheric loss process; calculated lifetimes of 2.9 d, ~13 d, > 28 d and 2.4 yr due to reactions with OH radical, NO$_3$ radical, O$_3$ and N$_2$O$_5$ (Arey et al. 1990)
16.1.5 AMIDES AND UREAS

16.1.5.1 Acetamide

Common Name: Acetamide
Synonym: ethanamide
Chemical Name: acetamide, acetic acid amine
CAS Registry No: 60-35-5
Molecular Formula: C₂H₅NO, CH₃CONH₂
Molecular Weight: 59.067
Melting Point (°C):
80.16 (Lide 2003)
Boiling Point (°C):
221 (Lide 2003)
Density (g/cm³ at 20°C):
0.9986 (78°C, Weast 1982–83)
1.159 (Verschueren, 1983)
Molar Volume (cm³/mol):
59.2 (calculated-density, Stephenson & Malanowski 1987)
66.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ: 7.62
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
56.1 (at bp, Riddick et al. 1986)
Enthalpy of Sublimation, ∆Hₛₐₜ (kJ/mol):
78.66 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₕₛ (kJ/mol):
17.707 (Riddick et al. 1986)
Entropy of Fusion, ∆Sₕₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕₛ = 56 J/mol K), F: 0.288 (mp at 80.16°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
975000 (20°C, Verschueren 1983)
408000 (20°C, Riddick et al. 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.61 (extrapolated-regression of tabulated data, temp range 65–222°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 14025.3/(T/K)] + 9.088352; temp range 65.0–222°C (Antoine eq., Weast 1972–73)
100 (Riddick et al. 1986)
log (P/kPa) = 8.24516 – 3282.80/(T/K); temp range 65–150°C (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 7.93409 – 2936.07/(T/K); temp range 65–bp (Antoine eq., Riddick et al. 1986)
2.44 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 10.9717 – 4050.1/(T/K); temp range 298–349 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 7.97099 – 1998.3/(–89.32 + T/K); temp range 381–492 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = –413.1683 + 8.1328 × 10⁻³/(T/K) + 172.9 log (T/K) – 0.16059·(T/K)² + 5.3892 × 10⁻⁵·(T/K)³; temp range 354–761 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
3.53 × 10⁻⁴ (calculated-P/C with selected values)
Octanol/Water Partition Coefficient, log K₀ₒₜₚ:
–1.09 (shake flask-radiochemical method, Cornford 1982)
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, $t_\frac{1}{2}$:

Volatile:

Photolysis:

Oxidation: photooxidation $t_\frac{1}{2} = 3.2–32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

Hydrolysis: overall rate constant $k_h = 5.5 \times 10^{-12}$ s$^{-1}$ with $t_h = 3950$ yr; acid rate constant $k_a = 8.36 \times 10^{-6}$ s$^{-1}$ and base rate constant $k_b = 5.5 \times 10^{-5}$ s$^{-1}$ at 25°C and pH 7 (Mabey & Mill 1978) acid rate constant $k = 0.03 [M \pm (H^+) \pm h]\text{ atm}$ and base rate constant $k = 0.17 [M \pm (OH^-) \pm h]\text{ atm}$ at pH 9 with first-order hydrolysis $t_h = 3950$ yr at pH 7 and 25°C, (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_\frac{1}{2} = 24–168$ h, based on aerobic aqueous screening test data (Malaney & Gerhold 1962, 1969; Urano & Kato 1986; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_\frac{1}{2} = 96–672$ 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: photooxidation $t_\frac{1}{2} = 3.2–32$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

Surface water: $t_\frac{1}{2} = 24–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_\frac{1}{2} = 48–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_\frac{1}{2} = 24–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
16.1.5.2 Acrylamide

\[
\begin{align*}
\text{O} & \quad \text{NH}_2 \\
\end{align*}
\]

Common Name: Acrylamide
Synonym: 2-propenamide
Chemical Name: acrylamide
CAS Registry No: 79-06-1
Molecular Formula: C₃H₅NO, CH₂=CHCONH₂
Molecular Weight: 71.078
Melting Point (°C): 84.5 (Lie 2003)
Boiling Point (°C): 192.5 (Lide 2003)
Density (g/cm³ at 20°C): 1.122 (30°C, Dean 1985)
Molar Volume (cm³/mol): 80.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Fusion, ΔH₈us (kJ/mol):
Entropy of Fusion, ΔS₈us (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₈us = 56 J/mol K), F: 0.261 (mp at 84.5°C)

Water Solubility (g/m³ or mg/L at 25°C):
2050000 (quoted, Verschueren 1983)
2150000 (30°C, Dean 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.616 (average, extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
\[
\log (P_\text{v}/\text{kPa}) = 7.395 - 3213/(T/K), \text{ temp range 357–413 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P_\text{v}/\text{kPa}) = 10.31055 - 3994.667/(T/K), \text{ temp range 373–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{mmHg}) = 17.0034 - 4.4434 \times 10^3/(T/K) - 1.7158 \log (T/K) + 2.0063 \times 10^{-6} \times (T/K) - 8.0394 \times 10^{-10} \times (T/K)^2; \text{ temp range 358–477 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pam³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kₐw:
–0.90 (shake flask, Fujisawa & Masuhara 1980, 1981)
–1.24 (calculated-HPLC-RT correlation, Fujisawa & Masuhara 1981)
–0.67 (shake flask, Log P Database, Hansch & Leo 1987)
–0.78 (recommended, Sangster 1989)
–0.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KₐA:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KₐC:
–0.969 (calculated-Kₐw, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:

Half-Lives in the Environment:
Surface water: measured rate constant k = (1.0 ± 0.1) × 10⁴ M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 5.4–5.8 and 22 ± 1°C, with t₁/₂ = 0.3 s at pH 7 (Yao & Haag 1991).
16.1.5.3 Benzamide

![Image of Benzamide structure]

Common Name: Benzamide  
Synonym: benzoylamide  
Chemical Name: benzamide  
CAS Registry No: 55-21-0  
Molecular Formula: C₇H₇NO, C₆H₅CONH₂  
Molecular Weight: 121.137

Melting Point (°C):  
127.3  
(Informe 2003)

Boiling Point (°C):  
290  
(Informe 2003)

Density (g/cm³ at 20°C):  
112.2  
(Informe 130°C, Stephenson & Malanowski 1987)
132.4  
(calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Fusion, ΔHᵢᵤₛ (kJ/mol):

Entropy of Fusion, ΔSᵢᵤₛ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSᵢᵤₛ = 56 J/mol K), F: 0.0992 (mp at 127.3°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

13500  
(Informe 20–25°C, shake flask-gravimetric method, Dehn 1917)
13499  
(Tsonopoulos & Prausnitz 1971)
13490  
(Windholz 1983)
13515  
(1 g in 74 mL, Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.00522  
(extrapolated, Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P_j/kPa) = 11.69847 - \frac{5062.899}{(T/K)}, \text{ temp range 325–342 K (solid, Antoine eq., Stephenson & Malanowski 1987)}
\]

Henry’s Law Constant (Pam³/mol at 25°C):

4.52 × 10⁻⁵  
(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log Kᵦₐₜₜ:

0.64  
(shake flask-UV, Fujita et al. 1964)
0.65  
(shake flask, Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1987)
0.66  
(shake flask-UV, Yaguzhinskii et al. 1973)
0.84  
(HPLC-k' correlation, Hammers et al. 1982)
0.64  
(shake flask-UV, Sotomatsu et al. 1987)
0.50  
(centrifugal partition chromatography CPC, Berthod et al. 1988)
0.81  
(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
0.64  
(recommended, Sangster 1989, 1993)
0.65  
(counter-current chromatography, Vallat et al. 1990)
0.65  
(CPC-RV correlation, El Tayar et al. 1991)
0.64  
(shake flask-GC, Alcorn et al. 1993)
0.64  
(recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

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

- 0.954; 1.301; 1.756 (sediment; Alfisol soil; Podzol soil, von Oepen et al. 1991)
- 1.46 (soil, quoted exptl., Meylan et al. 1992)
- 1.71 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 1.46 (soil, mean value, Kördel et al. 1993)
- 1.46 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.46; 1.71 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.87, 2.17, 1.12, 1.36, 1.645 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 1.46, 1.22; 2.18, 1.75, 1.88, 1.83, 1.31 (soil: quoted lit., calculated-$K_{OW}$; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:

Volatilization:

Photolysis:

Oxidation: aqueous photooxidation $t_1/2 = 960–7.4 \times 10^4$ h, based on measured rates for reaction with OH radical in water (Anbar et al. 1966; Dorfman and Adams 1973; selected, Howard et al. 1991);

- photooxidation $t_1/2 = 3.1 – 31$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Hydrolysis: not expected to be significant based on estimated half-lives for hydrolysis of acetamide of 261, 3950, and 46 yr at pH 5.7.9, respectively, which were calculated using experimental acid and base hydrolysis rate constants for acetamide (Mabey & Mill 1978; selected, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_1/2 = 48 – 360$ h, and aqueous anaerobic biodegradation $t_1/2 = 192 – 1400$ h, both based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_1/2 = 3.1 – 31$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Surface water: $t_1/2 = 48 – 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Ground water: $t_1/2 = 96 – 720$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Sediment:

- Soil: $t_1/2 = 48 – 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biota:
16.1.5.4 Urea

\[
\begin{align*}
\text{Common Name:} & \quad \text{Urea} \\
\text{Synonym:} & \quad \text{carbamide, carbonyldiamide, Aquacare, Aquadrate, Basodexam, Keratinamin, Nutraplus, Onychomal, Pastaron, Ureaphil, Ureophil, Ureaeparl} \\
\text{Chemical Name:} & \quad \text{urea, carbamide, carbonyldiamide} \\
\text{CAS Registry No:} & \quad 57-13-6 \\
\text{Molecular Formula:} & \quad \text{CH}_4\text{N}_2\text{O}, \text{H}_2\text{NCONH}_2 \\
\text{Molecular Weight:} & \quad 60.055 \\
\text{Melting Point (°C):} & \quad 133 \quad \text{(Lide 2003)} \\
\text{Boiling Point (°C):} & \quad \text{decompose (Weast 1982–83; Lide 2003)} \\
\text{Density (g/cm}^3\text{):} & \quad 1.323 \quad \text{(Weast 1982–83)} \\
\text{Dissociation Constant, pKa:} & \\
\text{Molar Volume (cm}^3\text{/mol):} & \quad 58.0 \quad \text{(calculated-Le Bas method at normal boiling point)} \\
\text{Enthalpy of Fusion,} \Delta H_{\text{fus}} \text{ (kJ/mol):} & \\
\text{Entropy of Fusion,} \Delta S_{\text{fus}} \text{ (J/mol K):} & \\
\text{Fugacity Ratio at 25°C (assuming} \Delta S_{\text{fus}} = 56 \text{ J/mol ± K), F:} & \quad 0.0872 \quad \text{(mp at 133°C)} \\
\text{Water Solubility (g/m}^3\text{ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):} & \\
975000^* & \quad \text{(shake flask, measured range 0–69.5°C, Speyers 1902)} \\
790000 & \quad \text{(20–25°C, shake flask-gravimetric method, Dehn 1917)} \\
1047000^* & \quad \text{(20°C, shake flask, measured range 0–70°C, Pinck & Kelly 1925)} \\
53.97 \text{ wt %}^* & \quad \text{(23.85°C, synthetic method, measured range 18.72–73.11°C, Shnidman & Sunier 1932)} \\
\log x = -609.8/(T/K) + 1.468; & \quad \text{temp range 20–70°C (synthetic method, Shnidman & Sunier 1932)} \\
0.4388^* & \quad \text{(60°C, mole fraction solubility, synthetic method, measured range 60–100°C, Kakinuma 1941)} \\
997400 & \quad \text{(Windholz 1983)} \\
1000000 & \quad \text{(Dean 1985; Budavari 1989)} \\
\text{Vapor Pressure (Pa at 25°C and reported temperature dependence equations):} & \\
1.61 \times 10^{-3} & \quad \text{(extrapolated-Antoine eq., Stephenson & Malanowski 1987)} \\
\log (P_2/kPa) = 9.565 – 4579/(T/K); & \quad \text{temp range 345–368 K (solid, Antoine eq., Stephenson & Malanowski 1987)} \\
\text{Henry’s Law Constant (Pam}^3\text{/mol):} & \\
\text{Octanol/Water Partition Coefficient,} \log K_{\text{OW}}: & \\
-1.09 & \quad \text{(Hansch & Leo 1979)} \\
-3.00 & \quad \text{(Kenaga & Goring 1980)} \\
-1.21, -1.79 & \quad \text{to} -0.62 \quad \text{(shake flask method: mean, range of mean values, OECD 1981)} \\
-1.54 & \quad \text{(shake flask-radiochemical method, Cornford 1982)} \\
-1.57 & \quad \text{(HPLC-RT correlation, Harnish et al. 1983)} \\
-1.56 & \quad \text{(shake flask, OECD 1981 Guidelines, Geyer et al. 1984)} \\
-1.66, -2.11 & \quad \text{(shake flask, Log P Database, Hansch & Leo 1987)} \\
-1.60 & \quad \text{(shake flask-UV, pH 7.4, Huang 1990)} \\
-2.11 & \quad \text{(from Medchem software value, Chessells et al. 1992)} \\
-2.11 & \quad \text{(recommended, Sangster 1993)} \\
-1.66 & \quad \text{(Hansch et al. 1995)}
Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.068 \hspace{1cm} (algae *chlorella fusca*, wet wt. basis, Geyer et al. 1984)
- −0.10 \hspace{1cm} (algae *chlorella fusca*, calculated-$K_{OW}$, Geyer et al. 1984)

Bioconcentration Factor, $\log BCF$:

- 0.50, 0.62 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 0.90 \hspace{1cm} (soil, calculated-MCI $'\chi'$, Sabljic et al. 1995)

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

- 0.50, 0.62 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 0.90 (soil, calculated-MCI $'\chi'$, Sabljic et al. 1995)

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

<table>
<thead>
<tr>
<th>TABLE 16.1.5.4.1</th>
<th>Reported aqueous solubilities of urea at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speyers 1902</td>
<td>Shnidman &amp; Sunier 1932</td>
</tr>
<tr>
<td>re-calcd by Pinck &amp; Kelly</td>
<td>synthetic method-heating -shake flask</td>
</tr>
<tr>
<td>$t/^\circ C$</td>
<td>$S/g \cdot m^{-3}$</td>
</tr>
<tr>
<td>----------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>0</td>
<td>674000</td>
</tr>
<tr>
<td>11.0</td>
<td>875000</td>
</tr>
<tr>
<td>19.8</td>
<td>975000</td>
</tr>
<tr>
<td>31.7</td>
<td>1310000</td>
</tr>
<tr>
<td>51.4</td>
<td>1930000</td>
</tr>
<tr>
<td>69.5</td>
<td>2530000</td>
</tr>
<tr>
<td>75°C</td>
<td>67.36</td>
</tr>
<tr>
<td>76.9</td>
<td>132.7</td>
</tr>
<tr>
<td>77.0</td>
<td>132.7</td>
</tr>
<tr>
<td>$\Delta H_{sol}/(kJ \cdot mol^{-1})$</td>
<td>61.76</td>
</tr>
<tr>
<td>25°C</td>
<td>673.11</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pinck &amp; Kelly 1925</th>
<th>mole fraction solubility expressed as: $\log x = \frac{A}{T} - \frac{B}{T}$; temp range 20–70°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/^\circ C$</td>
<td>$S/g \cdot m^{-3}$</td>
</tr>
<tr>
<td>----------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>0</td>
<td>670000</td>
</tr>
<tr>
<td>10.0</td>
<td>840000</td>
</tr>
<tr>
<td>20.0</td>
<td>1047000</td>
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<td>30.0</td>
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<td>39.7</td>
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<tr>
<td>50.0</td>
<td>2050000</td>
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<tr>
<td>50.6</td>
<td>2064000</td>
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<tr>
<td>60.0</td>
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<td>68.5</td>
<td>2950000</td>
</tr>
<tr>
<td>70.0</td>
<td>3146000</td>
</tr>
</tbody>
</table>

$\text{urea 1#} = \text{urea made by synthetic NH}_2 + \text{CO}_2 \text{ process—re-crystallized from water}$

$\text{urea 2#} = \text{urea made from calcium-cyanamid — re-crystallized from water and methanol}$
FIGURE 16.1.5.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for urea.
16.1.6 NITROSAMINES

16.1.6.1 N-Nitrosodimethylamine

Common Name: Dimethylnitrosoamine
Synonym: N-nitrosodimethylamine, N-methyl-N-nitrosomethanamine, nitrous dimethylamine
Chemical Name: dimethylnitrosoamine, N-nitrosodimethylamine
CAS Registry No: 62-75-9
Molecular Formula: C₂H₆N₂O, CH₃N(NO)CH₃
Molecular Weight: 74.081
Melting Point (°C):
Boiling Point (°C):
  152  (Lide 2003)
Density (g/cm³ at 20°C):
  1.005  (18°C, Verschueren 1983)
Molar Volume (cm³/mol):
  73.7  (10°C, Stephenson & Malanowski 1987)
  87.7  (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
  < 1.0  (Kollig 1993)
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):
  miscible  (Mivish et al. 1976)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
  1080  (Mabey et al. 1982)
  730  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  log (P_Pa/kPa) = 7.10632 – 2159.476/(T/K), temp range 309–423 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
  3.344  (calculated, Mabey et al. 1982)
Octanol/Water Partition Coefficient, log K_{OW}:
  0.06  (Radding et al. 1977)
  –0.57  (shake flask-UV, Singer et al. 1977)
  –0.68  (calculated-f const., Mabey et al. 1982)
  0.46  (30.5°C, shake flask-HPLC, Vera et al. 1992)
  0.76  (calculated, Kollig 1993)
  –0.57  (recommended, Sangster 1993)
  –0.57  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
  –0.96  (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
Sorption Partition Coefficient, log K_{OC}:
  –1.00  (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
  0.448  (calculated-K_{OW}, Kollig 1993)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatileization:
Photolysis: both aqueous and atmospheric photolysis $t_{1/2} = 0.5–1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

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; rate constants $k < 3600$ M$^{-1}$ h$^{-1}$ for singlet oxygen, and $k < 3600$ M$^{-1}$ h$^{-1}$ for peroxyl radical at 25°C (Mabey et al. 1982);

$k_{OH} = 3.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{O3} \leq 1 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Tuazon et al. 1984);
photooxidation $t_{1/2} = 25.4–254$ h in air, based on measured rate constant for the reaction with OH radical in air (Howard et al. 1991);
$k_{OH} = (2.53 – 3.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the gas-phase reactions with OH radical at 296–298 K (Atkinson 1989).

Biodegradation: aqueous aerobic $t_{1/2} = 504–4320$ h, based on aerobic soil die-away test data; and aqueous anaerobic $t_{1/2} = 2016–17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975; and Oliver et al. 1979; Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12}$ mL cell$^{-1}$ h$^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:
Air: $t_{1/2} = 0.5–1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991);
estimated photolysis $t_{1/2} \sim 5$ min, $t_{1/2} = 3$ d for reaction with OH radical and $t_{1/2} > 2$ yr for reaction with O$_3$ (Tuazon et al. 1984);
photooxidation $t_{1/2} = 25.4–254$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991).
Surface water: $t_{1/2} = 0.5–1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).
Groundwater: $t_{1/2} = 1008–8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: degradation $t_{1/2} \sim 3$ wk in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)
$t_{1/2} = 504–4320$ h, based on aerobic soil die-away test data (derived from data of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota:
16.1.6.2  \textit{N}-Nitrosodipropylamine

\[
\begin{tikzpicture}
  \node [align=center] (N) {\textit{N}\textnormal{-}};
  \node [align=center, below=0.3cm] (NO) {\textit{NO}};
\end{tikzpicture}
\]

Common Name: Di-\textit{n}-Propylnitrosoamine
Synonym: \textit{N}-nitrosodi-\textit{n}-propylamine, \textit{N}-nitroso-N-propyl-1-propanamine
Chemical Name: di-\textit{n}-propylnitrosoamine, \textit{N}-nitrosodi-\textit{n}-propylamine
CAS Registry No: 621-64-7
Molecular Formula: C_6H_{14}N_2O, CH_3CH_2CH_2N(NO)CH_2CH_2CH_3
Molecular Weight: 130.187
Melting Point (°C):
Boiling Point (°C):
\hspace{1cm} 206 \hspace{1cm} \text{(Lide 2003)}
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
\hspace{1cm} 176.5 \hspace{1cm} \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 (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), \(F\):
Water Solubility (g/m³ or mg/L at 25°C):
\hspace{1cm} 9900 \hspace{1cm} \text{(Mirvish et al. 1976)}
Vapor Pressure (Pa at 25°C):
\hspace{1cm} 53.33 \hspace{1cm} \text{(37°C, calculated-Troutin’s rule, Mabey et al. 1982)}
Henry’s Law Constant (Pam³/mol at 25°C):
\hspace{1cm} 0.638 \hspace{1cm} \text{(calculated-P/C, Mabey et al. 1982)}
\hspace{1cm} 0.355 \hspace{1cm} \text{(calculated-P/C, this work)}
Octanol/Water Partition Coefficient, \(\log K_{\text{OW}}\):
\hspace{1cm} 1.31 \hspace{1cm} \text{(calculated as per Leo et al. 1971 from Mirvish et al. 1976 data, Callahan et al. 1979)}
\hspace{1cm} 1.36 \hspace{1cm} \text{(shake flask-UV, Singer et al. 1977)}
\hspace{1cm} 1.49 \hspace{1cm} \text{(calculated-f const., Mabey et al. 1982)}
\hspace{1cm} 2.35 \hspace{1cm} \text{(30.5°C, shake flask-HPLC, Vera et al. 1992)}
\hspace{1cm} 2.45 \hspace{1cm} \text{(recommended, Sangster 1993)}
\hspace{1cm} 1.35 \hspace{1cm} \text{(Kollig 1993)}
\hspace{1cm} 1.36 \hspace{1cm} \text{(recommended, Hansch et al. 1995)}
Octanol/Air Partition Coefficient, \(\log K_{\text{OA}}\):
Bioconcentration Factor, \(\log BCF\):
\hspace{1cm} 0.99 \hspace{1cm} \text{(microorganisms-water, calculated-}K_{\text{OW}}, \text{Mabey et al. 1982)}
Sorption Partition Coefficient, \(\log K_{\text{OC}}\):
\hspace{1cm} 1.18 \hspace{1cm} \text{(sediment-water, calculated-}K_{\text{OW}}, \text{Mabey et al. 1982)}
\hspace{1cm} 1.09 \hspace{1cm} \text{(calculated-}K_{\text{OW}}, \text{Kollig 1993)}
Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{\frac{1}{2}}\):
Volatilization:
\hspace{1cm} \text{Photolysis: both aqueous and atmospheric photolysis } t_{\frac{1}{2}} = 0.17–1.0 \text{ h, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).}
Hydrolysis:
Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxo radical $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ at $25^\circ\text{C}$ (Mabey et al. 1982);

photooxidation $t_{1/2} = 2.66–26.6 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 504–4320 \text{ h}$, based on aerobic soil die-away test data, and aqueous anaerobic $t_{1/2} = 2016–17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biotransformation: rate constant for bacterial biotransformation $k \approx 3 \times 10^{-12} \text{ mL ± cell}^{-1} ± \text{ h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.66–26.6 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.17–1.0 \text{ h}$, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 1008–8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} \approx 3 \text{ wk}$ in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{1/2} = 504–4320 \text{ h}$, based on aerobic soil die-away test data (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota
16.1.6.3 DiphenylNitrosoamine

Common Name: DiphenylNitrosoamine
Synonym: N-nitrosodiphenylamine, N-nitroso-N-phenylbenzamine
Chemical Name: diphenylNitrosoamine, N-nitrosodiphenylamine
CAS Registry No: 86-30-6
Molecular Formula: C_{12}H_{10}N_{2}O, C_6H_5N(NO)C_6H_5
Molecular Weight: 198.219
Melting Point (°C):
- 66.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
- 151–153 (Windholz 1976; Callahan et al. 1979)
Density (g/cm^3 at 20°C):
- Molar Volume (cm^3/mol):
  - 220.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
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: 0.392 (mp at 66.5°C)
Water Solubility (g/m^3 or mg/L at 25°C):
- 35.1 (shake flask-LSC, Banerjee et al. 1980)
  - 40.0 (calculated-S, Mabey et al. 1982)
Vapor Pressure (Pa at 25°C):
- 13.33 (estimated, Mabey et al. 1982)
Henry’s Law Constant (Pam^3/mol at 25°C):
- 66.87 (calculated-P/C, Mabey et al. 1982)
Octanol/Water Partition Coefficient, log K_{ow}:
- 3.13 (shake flask-LSC, Banerjee et al. 1980;)
  - 3.13 (recommended, Sangster 1993)
  - 3.13 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
- 2.63 (microorganisms-water, calculated-K_{ow}, Mabey et al. 1982)
  - 2.34 (quoted, Isnard & Lambert 1988)
Sorption Partition Coefficient, log K_{oc}:
- 2.81 (sediment-water, calculated-K_{ow}, Mabey et al. 1982)
  - 2.84 (calculated-K_{ow}, Kollig 1993)
Environmental Fate Rate Constants, k, or Half-Lives, t\_1/2:
  - Volatilization:
  - Photolysis:
  - Hydrolysis:
Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxo radical $k < 3600 \text{ M}^{-1} \pm \text{ h}^{-1}$ at 25°C (Mabey et al. 1982); photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$ in air, based on measured rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991). 

Biodegradation: aqueous aerobic $t_{1/2} = 240 - 816 \text{ h}$, based on data from one soil-die-away test; a range was bracketed around the reported $t_{1/2} = 22 \text{ d}$ (Mallik & Tesfai 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 960 - 3264 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991). 

Biotransformation: rate constant for bacterial transformation $k = 1 \times 10^{-10} \text{ mL} \pm \text{ cell}^{-1} \pm \text{ h}^{-1}$ in water (Mabey et al. 1982). 

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (quoted, Howard et al. 1991). 

Surface water: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991). 

Groundwater: $t_{1/2} = 480 - 1632 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991). 

Sediment: 

Soil: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991). 

Biota:
16.1.7 HETEROCYCLIC COMPOUNDS

16.1.7.1 Pyrrole

- **Chemical Name:** pyrrole, 1H-pyrrole
- **CAS Registry No:** 109-97-7
- **Molecular Formula:** C₄H₄NH
- **Molecular Weight:** 67.090
- **Melting Point (°C):** –23.39 (Lide 2003)
- **Boiling Point (°C):** 129.79 (Lide 2003)
- **Density (g/cm³ at 20°C):**
  - 0.9691 (Weast 1982–83; Dean 1985)
  - 0.96985, 0.96565 (20°C, 25°C, Riddick et al. 1986)
- **Molar Volume (cm³/mol):**
  - 69.2 (20°C, calculated-density, Stephenson & Malanowski 1987)
  - 78.2 (calculated-Le Bas method at normal boiling point)
- **Dissociation Constant, pKₐ:**
  - –4.40 (Perrin 1972)
  - –3.80 (Riddick et al. 1986)
  - –4.10 (Sangster 1989)
- **Enthalpy of Vaporization, ΔHV (kJ/mol):**
  - 45.15, 38.75 (25°C, bp, Riddick et al. 1986)
- **Enthalpy of Fusion, ΔH_fus (kJ/mol):** 7.908 (Riddick et al. 1986)
- **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):**
  - 47000 (Dean 1985)
  - 45000 (Riddick et al. 1986)

- **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):**
  - 358285* (176.67°C, static-Bourdon gauge, measured range 176.67–271.11°C, Kobe et al. 1956)
  - 1102* (ebulliometry, extrapolated-Antoine eq., measured range 65.67–166°C, Scott et al. 1967; Osborn & Douslin 1968)

- **log (P/mmHg) = 7.30295 – 1507.015/(t/°C + 211.010); temp range 65.67–166°C (Antoine eq., ebulliometry, Scott et al. 1967)**

- **log [(P/atm) = [1 – 402.914 ± (T/K)] × 10^4] × 0.870073 – 5.43768 × 10^4 ± (T/K) + 4.16086 × 10^-7 ± (T/K)^2, temp range: 65.67–166°C (ebulliometric method, Cox eq., Scott et al. 1967)**

- **log (P/mmHg) = 7.30275 – 1506.877/(t/°C + 210.995), temp range 65.57–166°C (ebulliometric method, Antoine eq., Scott et al. 1967; Osborn & Douslin 1968)**

- **log [(P/atm) = [1 – 402.915 ± (T/K)] × 10^4] × 0.872196 – 5.54923 × 10^4 ± (T/K) + 4.30369 × 10^-7 ± (T/K)^2, temp range: 65.57–166°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)**

- **8386* (60.3°C, isotoniscope method, measured range 60.3–100.3°C, Eon et al. 1971)
- **1136** (calculated-Cox eq., Chao et al. 1983)

- **log (P/atm) = [1– 402.916/T(K)] × 10^4] × 0.880256 – 6.05913 × 10^4 ± (T/K) + 5.02726 × 10^-7 ± (T/K)^2; temp range: 250.0–635.0 K (Cox eq., Chao et al. 1983)**
Nitrogen and Sulfur Compounds

\begin{align*}
\text{Henry's Law Constant (Pa m}^3\text{/mol at 25°C):} \\
1.640 & \quad \text{(calculated-P/C with selected values)}
\end{align*}

Octanol/Water Partition Coefficient, log \(K_{ow}\) at 25°C or as indicated

\begin{align*}
0.75 & \quad \text{(shake flask-AS, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Leo 1979)} \\
0.62 & \quad \text{(HPLC-RV correlation, Garst 1984)} \\
0.82 & \quad \text{(23°C, shake flask-HPLC, De Voogt et al. 1988)} \\
0.80 & \quad \text{(23°C, TLC-RT correlation, De Voogt et al. 1990)} \\
0.75 & \quad \text{(recommended, Sangster 1989, 1993)} \\
0.75 & \quad \text{(recommended, Hansch et al. 1995)}
\end{align*}

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, \(t_\frac{1}{2}\):

Volatilization:

Photolysis:

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

\begin{align*}
\text{Volatilization:} \\
\text{Photolysis:} \\
\text{Oxidation: rate constant} \, k, \text{for reaction with OH radical, } k_{OH} \\
\text{with NO\(_3\) radical and } k_{ON} \text{ with O\(_3\)} \text{ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:} \\
k_{OH} &= (1.22 \pm 0.04) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K (relative rate method, Atkinson et al. 1984)} \\
k_{ON} &= 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate of 1.0 d}^{-1}, k_{OH} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate of 10 d}^{-1} \text{ and } k_{NO3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate of 1000 d}^{-1} \text{ (review, Atkinson \\
& Carter 1984)} \\
k_{ON} &= 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate of 1.0 d}^{-1}, k_{OH} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate of 5.2 d}^{-1} \text{ and } k_{NO3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with loss rate k = 1000 d}^{-1} \text{ (review, Atkinson 1985)} \\
k_{NO3} &= (4.9 \pm 1.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 \pm 1 K (relative rate method, Atkinson et al. 1985)} \\
k_{ON} &= 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with calculated tropospheric lifetime } \tau = 24 \text{ h}, k_{OH} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with } \tau(\text{calc}) = 2.3 \text{ h during daylight hours, } k_{NO3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with } \tau(\text{calc}) = 1.4 \text{ min during nighttime hours at room temp. (Atkinson et al. 1985)} \\
k_{OH} &= 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of 5.2 d}^{-1} \text{ at room temp. (Atkinson 1985)} \\
k_{OH} &= (1.03 \pm 0.06) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)} \\
k_{OH} &= 9.31 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Atkinson 1989)} \\
k_{OH} &= 1.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989)} \\
k_{OH}(\text{calc}) &= 287.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)} \\
\text{Hydrolysis:}
\end{align*}
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: calculated lifetimes of 2.3 h, 1.4 min and 24 h due to gas-phase reactions with OH radical (conc of $1 \times 10^6$ cm$^{-3}$ during daylight hours), NO$_3$ radical (conc of $2.4 \times 10^6$ cm$^{-3}$ during nighttime hours) and O$_3$ (clean tropospheric conc of $7.2 \times 10^{11}$ molecule cm$^{-3}$), respectively, at room temp. (Atkinson et al. 1985)

TABLE 16.1.7.1.1
Reported vapor pressures of pyrrole 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>
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<td>176.67</td>
<td>358285</td>
<td>65.671</td>
<td>9582</td>
<td>60.3</td>
<td>8386</td>
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<td>25007</td>
<td>60.3</td>
<td>8386</td>
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<td>106.096</td>
<td>47359</td>
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∆HV/(kJ mol$^{-1}$) = 41.84

Kobe et al. 1956
Scott et al. 1967
Eon et al. 1971

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FIGURE 16.1.7.1.1 Logarithm of vapor pressure versus reciprocal temperature for pyrrole.
16.1.7.2 Indole

Common Name: Indole
Synonym: benzo[b]pyrrole, 1-benzo[b]pyrrole, 1H-indole
Chemical Name: indole
CAS Registry No: 120-72-9
Molecular Formula: C₈H₇N
Molecular Weight: 117.149
Melting Point (°C):
52.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
254.0 (Weast 1982–83; Stephenson & Malanowski 1987)
253.6 (Lide 2003)
Density (g/cm³ at 20°C):
1.2200 (Weast 1982–83)
1.0643 (Dean 1985)
Molar Volume (cm³/mol):
133.4 (calculated-Le Bas method at boiling point)
Dissociation Constant, pKₐ:
−3.5, −3.62 (Perrin 1972)
−3.17 (Sangster 1989)
Enthalpy of Fusion, ΔHₑ𝑢ₙ (kJ/mol):
Entropy of Fusion, ΔSₑ𝑢ₙ J/mol K:
Fugacity Ratio at 25°C (assuming ΔSₑ𝑢ₙ = 56 J/mol K), F: 0.537 (mp at 52.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
3558 (shake flask-GC, Price 1976)
1874 (Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.24 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.369 – 1933.005/(254.707 + t°C); temp range 193.3–254.7°C (Antoine eq., Boublík et al. 1984)
1.565 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 10.3289 – 3916/(T/K); temp range 291–319 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 94.1625 – 6.9431 × 10³/(T/K) – 30.613-log (T/K) + 9.928 × 10⁻³-(T/K) + 1.7461 × 10⁻¹³·(T/K)²;
temp range 274–790 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pam³/mol at 25°C):
0.14 (calculated-P/C with selected values)
Octanol/Water Partition Coefficient, log Kₒₜₒₜₜ:
1.14 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
2.14 (shake flask-UV, Hansch & Anderson 1967)
2.25 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
2.00 (unpublished result, Leo et al. 1971)
2.00, 2.25, 2.13 (Hansch & Leo 1979)
1.66 (RP-HPLC-RT correlation, Veith et al. 1979a)
2.17 (RP-HPLC-RT correlation, Hanai & Hubert 1982)
2.14 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
Nitrogen and Sulfur Compounds

1.92 (inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
2.16 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.81 (HPLC-kin correlation, Eadsforth 1986)
2.16 (HPLC-RT correlation, Minick et al. 1988)
2.14 (recommended, Sangster 1989; 1993)
2.27 (23°C, shake flask-HPLC, De Voogt et al. 1988, 1990)
2.07 (HPLC-RT correlation, De Voogt et al. 1990)
2.19 (HPLC-RT correlation, Ritter et al. 1994)
2.14 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:
16.1.7.3 Pyridine

Common Name: Pyridine
Synonym:
Chemical Name: pyridine
CAS Registry No: 110-86-1
Molecular Formula: C₅H₅N
Molecular Weight: 79.101
Melting Point (°C):
 -41.7 (Lide 2003)
Boiling Point (°C): 115.23 (Lide 2003)
Density (g/cm³ at 20°C): 0.9819 (Weast 1982–83)
Molar Volume (cm³/mol):
80.6 (calculated-density, Rohrschneider 1973)
93.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.23 (pKₓ, Leo et al. 1971; Jori et al. 1983; Zachara et al. 1987)
5.198, 5.21, 5.22, 5.229 (Perrin 1972)
5.54 (UV, Yeh & Higuchi 1976)
5.23, 5.16 (quoted, shake flask-TN, Clarke 1984)
5.17 (pKₓH⁺, Dean 1985; Riddick et al. 1986)
5.21 (pKₓ, Sangster 1989)
Enthalpy of Vaporization, ΔHV (kJ/mol):
40.41, 36.39 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
7.414 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Andon & Cox 1952; Andon et al. 1954; Jori et al. 1983; Riddick et al. 1986)
miscible (Dean 1985; Zachara et al. 1987; Stephenson 1993a)
miscible (Yaws et al. 1990)
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):
2666* (24.8°C, summary of literature data, temp range –18.9 to 115.4°C, Stull 1947)
2520 (interpolated-regression of tabulated data, Stull 1947)
620, 2109 (0, 20°C, static method-tensimeter, Brown & Barbaras 1947)
2775* (ebulliometry, measured range 47.3–115.5°C, extrapolated-Antoine eq., Herington & Martin 1953)
log (P/mmHg) = 7.05811 – 1384.991/(216.296 + t°C); temp range 47.3–115.5°C (Antoine eq., ebulliometric measurements, Herington & Martin 1953)
2774* (gas saturation, measured range 20–40°C, Andon et al. 1954)
461637* (176.67°C, static-Bourdon gauge, measured range 176.67–343.33°C, Kobe et al. 1956)
log (P/mmHg) = 7.04162 – 1374.103/(215.014 + t°C); temp range 67.3–152.9°C (Antoine eq. ebulliometry, McCullough et al. 1957)
2763* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)
log (P/mmHg) = 7.04144 – 1373.990/(t/°C + 215.001); temp range 67.3–152.9°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)

log [(P/atm) = [1 – 399.384 ± (T/K)] × 10^4(0.856586 – 6.60597 × 10^4 ± (T/K) + 5.93625 × 10^7 ± (T/K)^2), temp range: 67.3–152.9°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)

2789 (calculated-Antoine eq., Cabani et al. 1971)

log (P/mmHg) = [-0.2185 × 9649.4/(T/K)] + 8.347670; temp range −18.9 to 115.4°C (Antoine eq., Weast 1972–73)

2767 (calculated-Cox eq., Chao et al. 1983)

log (P/atm) = [1– 388.399/(T/K)] × 10^{0.848882 – 6.09810 × 10 –4 ±( T / K) + 5.15399 × 10–7 ±( T / K )2}; temp range: 235.0–620.0 K (Cox eq., Chao et al. 1983)

2775, 2763 (extrapolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.18338 – 1385.39/(115.256 + t/°C); temp range 47.3–115.4°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)

log (P/kPa) = 6.16609 – 1373.826/(115.235 + t/°C) (Antoine eq. from reported exptl. data of McCullough et al. 1957, Boublik et al. 1984)

2763 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.04115 – 1373.80/(214.98 + t/°C); temp range 67–153°C (Antoine eq., Dean 1985, 1992)

2773 (Howard et al. 1986; quoted, Banerjee et al. 1990)

2700 (selected, Riddick et al. 1986)

log (P/kPa) = 6.18595 – 1386.683/(216.469 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

2770 (interpolated-Antoine eq. II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.17372 – 1379.953/(-57.436 + T/K); temp range 323–426 K (Antoine eq. I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.30308 – 1448.781/(-50.948 + T/K); temp range 296–353 K (Antoine eq. II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.16446 – 1373.263/(-58.18 + T/K); temp range 348–434 K (Antoine eq. III, Stephenson & Malanowski 1987)

log (P/kPa) = 6.284 – 1455.584/(-48.272 + T/K); temp range 431–558 K (Antoine eq. IV, Stephenson & Malanowski 1987)

log (P/kPa) = 7.25663 – 2578.625/(115.604 + T/K); temp range 552–620 K (Antoine eq. V, Stephenson & Malanowski 1987)

2773, 1653 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

2573* (24.82°C, ebulliometry, measured range 23.55–116.23°C, Łencka 1990)

ln (P/kPa) = 14.1480 – 3132.3/(T/K) – 59.179; temp range 295.7–388.4 K (ebulliometric measurements, Antoine eq., Łencka 1990)

log (P/mmHg) = 33.5541 – 3.1318 × 10^3/(T/K) – 8.8646-log (T/K) + 7.1293 × 10^-12·(T/K) + 2.2813 × 10^-6·(T/K)^2; temp range 232–620 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.895 (volatility ratio-transpiration method, Andon et al. 1954)

0.900 (exptl., Hine & Mookerjee 1975)

0.595, 0.766 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.114 (modified gas-stripping, Hawthorne et al. 1985)

1.120 (computed, Yaws et al. 1991)

0.305 (calculated-molecular structure, Russell et al. 1992)

27.78 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = -1.508 – 128/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.65 (shake flask-UV, Iwasa et al. 1965)

0.64 (Gehring et al. 1967)

0.65, 0.64 (Leo et al. 1971; Hansch & Leo 1979)

0.66 (HPLC-RT correlation, Mirrlees et al. 1976)

0.63 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

0.63 (shake flask-titration, Clarke 1984; Clarke & Cahoon 1987)

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0.63 ± 0.06 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.62 (shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.63 (shake flask-potentiometric titration, Clarke 1984)
0.54 (calculated- activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.28 (HPLC-k′ correlation, Eadsforth 1986)
0.79 (calculated-γ from UNIFAC, Banerjee & Howard 1988)
0.70 (shake flask-CPC, Berthod et al. 1988)
0.63 (shake flask-HPLC at pH 7, De Voogt et al. 1988, 1990)
0.65 (recommended, Sangster 1989, 1993)
0.70 (RP-TLC-RT correlation, De Voogt et al. 1990)
0.65 (shake flask-UV, Yamagami et al. 1990)
0.60 (pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

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

-1.805 (estimated of Anvil Points subsurface materials, Zachara et al. 1987)
-2.541 (estimated of Loring subsurface materials, Zachara et al. 1987)
0.340 (calculated-$K_{OW}$, Kollig 1993)

Environmental Fate Rate Constants, k, 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:

Photooxidation $t_\frac{1}{2} = 14.7–24.4$ yr in water, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (4.9 ± 0.4) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere; $k_{O3} < 1.1 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with atmospheric lifetimes of > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere at room temp. (relative rate method, Atkinson et al. 1987)

$k_{OH} = (0.494 - 0.256) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296–297 K (review, Atkinson 1989)

$k_{OH(calc)} = 0.45 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aqueous aerobic $t_\frac{1}{2} = 24–168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_\frac{1}{2} = 168–672$ h, based on anaerobic acclimated screening test data (Naik et al. 1972; selected, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp. and > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere, based on the gas-phase reaction with O$_3$ (calculated rate constant) in air at room temp. (Atkinson et al. 1987);

photooxidation $t_\frac{1}{2} = 128–1284$ h, based on measured rate data for the reaction with hydroxyl radical in air (selected, Howard et al. 1991).

Surface water: photooxidation $t_\frac{1}{2} = 14.7–24.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

$\text{t}_\frac{1}{2} = 24–168$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_\frac{1}{2} = 48–336$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: disappears in less than 7 d in soil suspensions (Sims & O’Loughlin 1989);
$t_{1/2} = 24–168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; selected, Howard et al. 1991).

**Biota:**

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** McCullough et al. 1957 **
comparative ebulliometry

** Osborn & Douslin 1968 **
ebulliometry

** Lencka 1990 **
ebulliometry

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**FIGURE 16.1.7.3.1** Logarithm of vapor pressure versus reciprocal temperature for pyridine.
16.1.7.4 2-Methylpyridine

Common Name: 2-Methylpyridine
Synonym: α-picoline, 2-picoline
Chemical Name: 2-methylpyridine, α-picoline
CAS Registry No: 109-06-8
Molecular Formula: C₅H₄NCH₃
Molecular Weight: 93.127
Melting Point (°C):
-66.68 (Lide 2003)
Boiling Point (°C):
129.38 (Lide 2003)
Density (g/cm³ at 20°C):
0.9443 (Weast 1982–83)
0.9444, 0.93981 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
98.6 (20°C, calculated-density)
115.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.957, 6.06 (Perrin 1972)
5.97 (pKₐ, 20°C, Weast 1982–83)
6.00 (pKₐ +, Riddick et al. 1986; quoted, Howard 1990)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
42.919, 36.271 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
9.724 (Riddick et al. 1986)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Andon & Cox 1952)
miscible (Riddick et al. 1986; Yaws et al. 1990)
miscible (Stephenson 1993a)
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):
1370* (interpolated-regression of tabulated data, temp range –11.0 to 128.8°C, Stull 1947)
308, 1140 (0, 20.3°C, static method-tensimeter, Brown & Barbaras 1947)
1277 (manometry, calculated-Antoine eq., Hopke & Sears 1951)
1496* (ebulliometry, extrapolated-Antoine eq., measured range 64.3–130°C, Herington & Martin 1953)
log (P/mmHg) = 7.03450 – 1417.578/(211.874 + t/°C); temp range 64.3–130°C (ebulliometric measurements, Antoine eq., Herington & Martin 1953)
1496 (calculated-Antoine eq., Andon et al. 1954)
19920* (79.794°C, comparative ebulliometry, measured range 79.8–168°C, Scott et al. 1963a)
log (P/mmHg) = 7.03202 – 1415.494/(t/°C + 211.589); temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Scott et al. 1963a)
1493 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)
log (P/mmHg) = 7.03192 – 1415.424/(t/°C + 211.589); temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)
\[
\log \left[ \frac{P}{\text{atm}} \right] = [1–402.536 \pm (T/K)] \times 10^\left\{0.866637 – 6.80114 \times 10^{-4} \pm (T/K) + 6.00534 \times 10^{-7} \pm (T/K)^2\right\}, \\
\text{temp range: 79.8–168°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)}
\]
log (P/mmHg) = \left[ -0.2185 \times 9933.2 / (T/K) \right] + 8.290910; \text{ temp range } -11.0 \text{ to } 128.8^\circ C \text{ (Antoine eq., Weast 1972–73)}

1500 \quad \text{(calculated-Cox eq., Chao et al. 1983)}

log (P/atm) = \left[ 1 - 402.320 / (T/K) \right] \times 10^{0.887914 - 7.70705 \times 10^{-4} \pm (T/K) + 6.85261 \times 10^{-7} \pm (T/K)^2}; \text{ temp range: } 215.0 \text{–} 620.0 \text{ K (Cox eq., Chao et al. 1983)}

1067 \quad \text{(20°C, Verschueren 1983)}

1494, 1498 \quad \text{(extrapolated-Antoine equations, Boublik et al. 1984)}

log (P/kPa) = \left[ 6.16509 - 1421.237 / (211.286 + t/°C) \right]; \text{ temp range } 64.363 \text{–} 130.04^\circ C \text{ (Antoine eq. from reported exppl. data of Herington & Martin 1953, Boublik et al. 1984)}

1067 \quad \text{(calculated-Antoine equations, Boublik et al. 1984)}

log (P/kPa) = \left[ 6.15940 - 1417.578 / (211.874 + t/°C) \right]; \text{ temp range } 79.79 \text{–} 168.36^\circ C \text{ (Antoine eq. from reported exppl. data of Scott et al. 1963, Boublik et al. 1984)}

log (P/kPa) = \left[ 6.15718 - 1415.663 / (211.617 + t/°C) \right]; \text{ temp range } 64.363 \text{–} 130.04^\circ C \text{ (Antoine eq. from reported exppl. data of Scott et al. 1963, Boublik et al. 1984)}

1494 \quad \text{(extrapolated-Antoine eq., Dean 1985, 1992)}

log (P/mmHg) = \left[ 7.0324 - 1421.73 / (211.63 + t/°C) \right]; \text{ temp range: } 80 \text{–} 168^\circ C \text{ (Antoine eq., Dean 1985, 1992)}

1333 \quad \text{(Riddick et al. 1986)}

log (P/kPa) = \left[ 6.15526 - 1415.29 / (211.63 + t/°C) \right]; \text{ temp range } 90 \text{–} 168^\circ C \text{ (Antoine eq., Dean 1985, 1992)}

1386 \quad \text{(extrapolated-Antoineeq., Stephenson & Malanowski 1987)}

log (P/kPa) = \left[ 5.2309 - 1164.1 / (T/K) \right]; \text{ temp range } 295.7 \text{–} 388.4^\circ K (Antoine eq., Łencka 1990)

ln (P/kPa) = \left[ 14.1560 - 3249.15 / (T/K) - 9.0927 \cdot \log (T/K) - 3.6324 \times 10^{-10} \cdot (T/K)^2 \right]; \text{ temp range } 206 \text{–} 621^\circ K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):

1.010 \quad \text{(measured volatility ratio-transpiration method, Andon et al. 1954)}

1.010 \quad \text{(exptl., Hine & Mookerjee 1975)}

0.821, 0.749 \quad \text{(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)}

2.90 \quad \text{(computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)}

30.22 \quad \text{(20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)}

\log K_{AW} = \left[ -0.700 - 354 / (T/K) \right]; \text{ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)}

Octanol/Water Partition Coefficient, \log K_{OW}:

0.52 \quad \text{(HPLC-RT correlation, Schultz & Moulton 1985)}

1.11 \quad \text{(shake flask, Log P Database, Hansch & Leo 1987)}

1.11 \quad \text{(shake flask-UV, Yamagami et al. 1990)}

1.11 \quad \text{(recommended, Sangster 1989; 1993)}

1.11 \quad \text{(recommended, Hansch et al. 1995)}

Octanol/Air Partition Coefficient, \log K_{OA}:

Bioconcentration Factor, \log BCF:

0.602 \quad \text{(calculated-K_{OW}, Lyman et al. 1982)}

Sorption Partition Coefficient, \log K_{OC}:

Environmental Fate Rate Constants, \k, or Half-Lives, \text{t}_1/2:
Volatilization: using Henry’s law constant, \( t_{1/2} = 88 \text{ h} \) for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Howard 1990).

Photolysis:
Oxidation: photooxidation \( t_{1/2} = 11.2 \text{ d} \) in air, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k\(_1\)) and Elimination (k\(_2\)) Rate Constants:

**Half-Lives in the Environment:**

- **Air:** \( t_{1/2} = 11.2 \text{ d} \), based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).
- **Surface water:** estimated \( t_{1/2} = 1.0 \text{ d} \) for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
- **Groundwater:**
- **Sediment:**
- **Soil:**
- **Biota:**

### TABLE 16.1.7.4.1

**Reported vapor pressures of 2-methylpryridine at various temperatures and the coefficients for the vapor pressure equations**

| \( T/°C \) | \( P/\text{Pa} \) | \( \log P = A – B/(T/K) \) | \( \ln P = A – B/(T/K) \) | \( \log P = A – B/(C + T/K) \) | \( 
\log P = A – B/(C + t/°C) \) | \( 
\log P = A – B/(T/K) – C·\log(T/K) \) |
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**Stull 1947**

**Herington & Martin 1953**

**Scott et al. 1963(a)**

**Lencka 1990**

**summary of literature data**

**ebulliometry**

**comparative ebulliometry**

**ebulliometry**

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### TABLE 16.1.7.4.1 (Continued)

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### FIGURE 16.1.7.4.1

2-Methylpyridine: vapor pressure vs. 1/T

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FIGURE 16.1.7.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpyridine.
3-Methylpyridine

Common Name: 3-Methylpyridine
Synonym: β-picoline, 3-picoline
Chemical Name: 3-methylpyridine, β-picoline
CAS Registry No: 108-99-6
Molecular Formula: C₅H₄NCH₃
Molecular Weight: 93.127
Melting Point (°C):
-18.14 (Lide 2003)
Boiling Point (°C):
144.14 (Lide 2003)
Density (g/cm² at 20°C):
0.9443 (Weast 1982–83)
0.9566 (Riddick et al. 1986)
Molar Volume (cm³/mol):
97.35 (20°C, calculated-density)
115.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.67, 5.703 (Perrin 1972)
5.68 (pKₐ, 20°C, Weast 1982–83; pKₐ+, protonated cation + 1, Dean 1985)
5.75 (pKₐH⁺, Riddick et al. 1986)
5.65 (pKₐ, Sangster 1989)
Enthalpy of Vaporization, ∆HV (kJ/mol):
45.233, 37.323 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₕ fus (kJ/mol):
14.18 (Riddick et al. 1986)
Entropy of Fusion, ∆Sₕ fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕ fus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Andon & Cox 1952; Andon et al. 1954; Yaws et al. 1990)
miscible (Riddick et al. 1986; Howard 1993)
miscible (Stephenson 1993a)
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):
150.7, 594.6 (0, 20°C, static method-tensimeter, Brown & Barbaras 1947)
794* (ebulliometry, extrapolated-Antoine eq., Hertington & Martin 1953)
log (P/mmHg) = 7.03247 – 1469.894/(209.907 + t°C); temp range 81.2–145.1°C (ebulliometric measurements, Antoine eq., Hertington & Martin 1953)
794 (calculated-Antoine eq., Andon et al. 1954)
9582* (74.036°C, comparative ebulliometry, measured range 74.036–184.568°C, Scott et al. 1963b)
log (P/mmHg) = 7.05375 – 1484.208/(t°C + 211.532), temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Scott et al. 1963b)
811 (ebulliometry, calculated-Antoine eq., Osborn & Dousslin 1968)
log (P/mmHg) = 7.30275 – 1506.877/(t°C + 210.995), temp range: 74–185°C, (ebulliometric measurements, Antoine eq., Osborn & Dousslin 1968)
log [(P/atm) = [1 – 417.287 ± (T/K)] x 10ⁿ(0.854256 – 6.02835 x 10⁻⁴ ± (T/K)) + 5.00169 x 10⁻⁷ ± (T/K)²], temp range: 74–185°C (ebulliometric method, Cox eq., Osborn & Dousslin 1968)
806 (calculated-Cox eq., Chao et al. 1983)
\[
\log (P/\text{atm}) = [1 - 417.217/(T/K)] \times 10^4\{0.865977 - 6.48542 \times 10^4 \pm (T/K) + 5.41256 \times 10^{-7} \pm (T/K)^2\}; \text{ temp range: } 255.0 - 645.0 \text{ K (Cox eq., Chao et al. 1983)}
\]

796, 800 (extrapolated-Antoine equations, Boublik et al. 1984)

\[
\log (P/\text{kPa}) = 6.16152 - 1472.639/(210.214 + t/\degree C); \text{ temp range } 81.3 - 145.1 \degree C (\text{Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984})
\]

\[
\log (P/\text{kPa}) = 6.17577 - 1482.229/(211.305 + t/\degree C); \text{ temp range } 74.03 - 184.6 \degree C (\text{Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984})
\]

800 (extrapolated-Antoine eq., Dean 1985, 1992)

\[
\log (P/\text{mmHg}) = 7.05021 - 1481.78/(211.25 + t/\degree C); \text{ temp range } 74 - 185 \degree C (\text{Antoine eq., Dean 1985, 1992})
\]

1333 (Riddick et al. 1986)

\[
\log (P/\text{kPa}) = 6.15737 - 1469.894/(209.907 + t/\degree C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

802 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/\text{kPa}) = 6.17593 - 1482.943/(-61.705 + T/K); \text{ temp range } 347 - 458 \text{ K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 6.17791 - 1484.285/(-61.554 + T/K); \text{ temp range } 347 - 458 \text{ K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 6.18988 - 1491.897/(-60.745 + T/K); \text{ temp range } 374 - 381 \text{ K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 6.16648 - 1476.25/(-62.502 + T/K); \text{ temp range } 374 - 458 \text{ K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 6.38586 - 1659.184/(-38.176 + T/K); \text{ temp range } 450 - 570 \text{ K (Antoine eq.-VI, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 7.57549 - 3151.52/(161.352 + T/K); \text{ temp range } 561 - 645 \text{ K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{mmHg}) = 35.2679 - 3.4364 \times 10^3/(T/K) - 9.3555 \log (T/K) - 1.3286 \times 10^{-10}(T/K) + 2.0461 \times 10^{-6}(T/K)^2; \text{ temp range } 255 - 645 \text{ K (vapor pressure eq., Yaws 1994)}
\]

\[
\text{Henry’s Law Constant (Pa·m}^3\text{/mol at 25°C or as indicated):}
\]

0.788 (volatility ratio-transpiration method, Andon et al. 1954)

0.784; 0.637; 0.749 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

1.836 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

12.69 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

\[
\log K_{\text{AW}} = -0.826 - 348/(T/K) \text{ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, \(\log K_{\text{OW}}\):

1.20 (HPLC-RT correlation, Mirrlees et al. 1976)

1.20 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

1.19 (HPLC-RT correlation, Lewis et al. 1983)

1.18 ± 0.01 (HPLC-RV correlation-ALPM, Garst 1984; Garst & Wilson 1984)

1.20 (shake flask, Log P Database, Hansch & Leo 1985, 1987)

1.20 (recommended, Sangster 1989, 1993)

1.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \(\log K_{\text{OA}}\):

Bioconcentration Factor, \(\log BCF\):

0.699 (calculated-\(K_{\text{OW}}\), Lyman et al. 1982; quoted, Howard 1993)

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

2.029 (soil, calculated-\(K_{\text{OW}}\), Lyman et al. 1982; quoted, Howard 1993)

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

Volatilization:

Photolysis:

Oxidation: estimated photooxidation rate constant \(k = 1.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) for the vapor-phase reaction with \(5 \times 10^3\) hydroxyl radicals/cm\(^3\) in air at 25°C which corresponds to an atmospheric half-life of 11 d (Atkinson 1987; quoted, Howard 1993).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:
Air: atmospheric t½ = 11 d from estimated photooxidation rate constant k = 1.43 × 10⁻¹² cm³ ± molecule⁻¹ s⁻¹ for the vapor-phase reaction with 5 × 10⁹ hydroxyl radicals/cm³ in air at 25°C (Atkinson 1987; quoted, Howard 1993).
Surface water: estimated t½ = 1.0 d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

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<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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ΔH_v/(kJ mol⁻¹) = 37.76

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<td>310101</td>
</tr>
</tbody>
</table>

bp/°C 144.143

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FIGURE 16.1.7.5.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methylpyridine.
16.1.7.6 2,3-Dimethylpyridine

![Chemical Structure](image)

**Common Name:** 2,3-Dimethylpyridine  
**Synonym:** 2,3-lutidine  
**Chemical Name:** 2,3-dimethylpyridine, 2,3-lutidine  
**CAS Registry No:** 583-61-9  
**Molecular Formula:** C₇H₉N, C₅H₃N(CH₃)₂  
**Molecular Weight:** 107.153  

**Melting Point (°C):**  
-15.5 (Stephenson & Malanowski 1987)

**Boiling Point (°C):**  
161.12 (Lide 2003)

**Density (g/cm³ at 20°C):**  
0.9461, 0.9421 (20°C, 25°C, Coulson et al. 1959)  
0.9319 (25°C, Weast 1982–83)

**Molar Volume (cm³/mol):**  
115.0 (calculated-density, Stephenson & Malanowski 1987)  
135.9 (calculated-Le Bas method at normal boiling point)

**Dissociation Constant, pK:**  
6.70 (20°C, Perrin 1972)  
6.57 (pKₐ, Weast 1982–83)

**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: 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):**  
104000* (20°C, shake flask-GC, measured range 16–90°C, Stephenson 1993a)

**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):**  
366.6, 922.6, 7119 (25, 40, 81.2°C, calculated-empirical method with bp and Antoine eq., Andon et al. 1954)  
346.4* (ebulliometry, extrapolated-Antoine eq., measured range 99.5–162.4°C, Coulson et al. 1959)  
log (P/mmHg) = 7.05075 – 152.935/(205.499 + t°C); temp range 99.5–162.4°C (Antoine eq., ebulliometry, Coulson et al. 1959)

359.0 (calculated-Cox eq., Chao et al. 1983)  
log (P/atm) = [1– 434.216/(T/K)] × 10⁵[0.881714 – 6.74484 × 10⁻⁴ ± (T/K) + 5.55055 × 10⁻² ± (T/K)²]; temp range: 260.0–655.0 K (Cox eq., Chao et al. 1983)

425.5 (extrapolated-Antoine eq., Boublík et al. 1984)  
log (P/kPa) = 6.45509 – 1739.902/(229.887 + t°C); temp range 155.3–162.4°C (Antoine eq. from reported exptl. data of Coulson et al. 1959, Boublík et al. 1984)

352.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P/kPa) = 6.18881 – 1538.772/(-66.477 + T/K); temp range; 372–476 K (Antoine eq., Stephenson & Malanowski 1987)

457 (extrapolated-Antoine eq., Dean 1992)  
log (P/mmHg) = 7.447 – 1832.6/(240.1 + t°C); temp range 155–162°C (Antoine eq., Dean. 1992)  

**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):**  
0.725 (volatility ratio-transpiration method, Andon et al. 1954)  
0.732 (exptl., Hine & Mookerjee 1975)
0.859, 0.732 (calculated.-group contribution, bond contribution, Hine & Mookerjee 1975)
21.01 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
\[ \log K_{\text{aw}} = 0.039 - 617/(T/K) \] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):

Octanol/Air Partition Coefficient, \( \log K_{\text{oa}} \):

Bioconcentration Factor, \( \log BCF \):

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

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

Half-Lives in the Environment:
Surface water: estimated \( t_{\frac{1}{2}} = 13.0 \text{ d} \) for dimethylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

### Table 16.1.7.6.1
Reported aqueous solubilities and vapor pressures of 2,3-dimethylpyridine at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
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<td>Stephenson 1993a</td>
<td>Coulson et al. 1959</td>
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<tr>
<td>step flask-GC/TC</td>
<td>ebulliometry</td>
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<tr>
<td>( t/\circ C )</td>
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</table>

\[ \Delta H_v = 41.07 \text{ kJ/mol} \]

Antoine eq.

\[ \log P = A - \frac{B}{C + t/\circ C} \]

\( P/\text{mmHg} \)

A 7.05075
B 1528.935
C 205.499
FIGURE 16.1.7.6.1 Logarithm of mole fraction solubility (ln $x$) versus reciprocal temperature for 2,3-dimethylpyridine.

FIGURE 16.1.7.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylpyridine.
16.1.7.7 Quinoline

Common Name: Quinoline
Synonym: benzo[b]-pyridine, 1-benzazine
Chemical Name: quinoline
CAS Registry No: 91-22-5
Molecular Formula: C₉H₇N
Molecular Weight: 129.159
Melting Point (°C):
-14.78 (Lide 2003)
Boiling Point (°C):
237.16 (Lide 2003)
Density (g/cm³ at 20°C):
1.0929 (Weast 1982–83)
1.09771, 1.08579 (15, 30°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
118.1 (calculated-density, Rohrschneider 1973)
144.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
4.80 (pKₐ, protonated cation + 1, Dean 1985)
4.94 (pK⁺, Riddick et al. 1986)
4.87 (pK⁺, Sangster 1989)
Enthalpy of Vaporization, ∆Hv (kJ/mol):
49.71 (at bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
10.79 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), 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):
6110 (Albersmeyer 1958)
6840 (shake flask-HPLC/UV, Fu & Luthy 1985, 1986)
6386* (20.35°C, equilibrium cell-GC, measured range 20.35–225°C, Leet et al. 1987)
5426 (centrifuge-HPLC at pH 7 and pH 8, Matzner et al. 1991)
8400, 6600 (20°C, 30°C, shake flask-GC, Stephenson 1993a)
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):
15.51* (extrapolated-regression of tabulated data, temp range 59.7–237.7°C, Stull 1947)
1.213 (extrapolated, Maczynski & Maczynska 1965)
ln (P/mmHg) = 20.96 – 6993.2/(T/K); temp range: 290.0–780.0 K (Cox eq., Chao et al. 1983)
11.04 (extrapolated-Antoine eq., Boublik et al. 1984)
\[
\log (P/kPa) = 5.94201 - 1668.355/(186.212 + t/°C), \text{ temp range } 164.7-237.9°C \text{ (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

11.05 (extrapolated-Antoine eq., Dean 1985, 1992)

\[
\log (P/mmHg) = 6.81759 - 1668.73/(186.26 + t/°C), \text{ temp range } 164-238°C \text{ (Antoine eq., Dean 1985, 1992)}
\]

1.21 (recommended, Neely & Blau 1985)

12.8 (Howard et al. 1986)

11.2 (Riddick et al. 1986)

\[
\log (P/kPa) = 5.92679 - 1656.30/(184.78 + t/°C); \text{ temp range not specified} \text{ (Antoine eq., Riddick et al. 1986)}
\]

42120* (472.85 K, vapor-liquid equilibrium, measured range 472.85–548.05 K, Klara et al. 1987)

\[
\log (P/kPa) = 14.4961 - 4390.0/(65.19 + T/K); \text{ temp range } 472.85–548.05 K \text{ (vapor-liquid equilibrium, Klara et al. 1987)}
\]

\[
\log (P/L/kPa) = 5.92679 - 1656.3/(–88.37 + T/K); \text{ temp range } 433–511 K \text{ (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P/L/kPa) = 7.15102 – 2846.253/(41.795 + T/K); \text{ temp range } 463–794 K \text{ (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

6.145 (calculated-solvatochromic parameters, Banerjee et al. 1990)

\[
\log (P/mmHg) = 76.5432 – 5.7748 \times 10^3/(T/K) – 24.619\log (T/K) + 8.4666 \times 10^{-3}\cdot(T/K) + 3.5586 \times 10^{-13}\cdot(T/K)^2; \text{ temp range } 258–782 K \text{ (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C):

0.0253 (calculated-P/C, Smith & Bomberger 1980)

0.026 (calculated-P/C, Mackay 1985)

0.168 (calculated-P/C, Meylan & Howard 1991)

0.0697 (estimated-bond contribution, Meylan & Howard 1991)

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

2.03 (shake flask-UV, Iwasa et al. 1965)

2.06 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

2.03 (Schultz et al. 1970)

2.04 (HPLC-RT correlation, Mirrlees et al. 1976)

2.04 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

2.02 (Hansch & Leo 1979)

2.01 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)

1.88 (HPLC-k’ correlation, Haky & Young 1984)

2.20 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

2.10 (shake flask-HPLC, De Voogt et al. 1988, 1990)

2.09 (28°C, shake flask-UV at pH 7.4, Go & Ngiam 1988)

2.03 (recommended, Sangster 1989, 1993)

2.10, 2.15 (HPLC-RT correlation, shake flask-electrometric titration, Slater et al. 1994)

2.03 (recommended, Hansch et al. 1995)

2.17 ± 0.66, 2.33 ± 0.56 (HPLC-k’ correlation: ODS–65 column, Diol–35 column, Helweg et al. 1997)

1.91 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

1.04 (Coyote Creek sediment with organic content of 1.9%, Smith et al. 1978)

1.96, 2.10, 1.67, 1.72 (estimated-K_{ow} Karickhoff 1985)

1.42, 1.62 (estimated-S, Karickhoff 1985)

2.20 (best estimate, Karickhoff 1985)

0.251 (estimated Anvil Points subsurface materials, Zachara et al. 1987)

–1.516 (estimated Loring subsurface materials, Zachara et al. 1987)

2.89; 3.05 (humic acid, HPLC-k’ correlation; quoted lit., Nielsen et al. 1997)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 7000$ h in stream, $t_{1/2} = 35000$ h in eutrophic pond and $t_{1/2} = 28000$ h in eutrophic lake and oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978).

Photolysis:

$\k = 7.8 \times 10^{-7}$ s$^{-1}$, assuming exposed to 12-h sunlight per day in June, photolysis $t_{1/2} = 1200$ h in stream, $t_{1/2} = 3000$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(aq.) = 3.6 \times 10^{-7}$ s$^{-1}$ for summer with $t_{1/2} = 535$ h and $k = 5.0 \times 10^{-8}$ s$^{-1}$ for winter with $t_{1/2} = 3851$ h both at pH 6.9 and under sunlight at 40°N (Mill et al. 1981; quoted, Howard et al. 1991)

$\text{photolytic } t_{1/2} = 550$ h in aquatics (Haque et al. 1980)

$\text{photolytic } t_{1/2} = 5$–12 d for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

$k = 2.8$ M$^{-1}$ s$^{-1}$ for the reaction with RO$_2$ radical with $t_{1/2} > 10^4$ h in stream, eutrophic pond and lake and oligotrophic lake, based on RO$_2$ concentration of $10^{-9}$ M on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(aq.) = 3.5 \times 10^{-7}$ s$^{-1}$ with $t_{1/2} = 548$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; $k(aq.) = 2.8$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

First-order photodegradation $k = 8.0 \times 10^{-6}$ s$^{-1}$ at 313 nm of in organic-free water with $t_{1/2} = 24.0$ h and $k = 8.4 \times 10^{-6}$ s$^{-1}$ in lake water with $t_{1/2} = 23$ h both saturated with air (Kochany & Maguire 1994)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$\text{Half-Lives in the Environment: }$

Air: $t_{1/2} = 10$ – 99 h, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991);

Surface water: half-life for all processes, except for dilution: $t_{1/2} = 0.5$ h in stream, eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978); half-life for all processes, including for dilution: $t_{1/2} = 0.28$ h in stream, $t_{1/2} = 0.5$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

$\text{Biodegradation }$ $t_{1/2} = 5$ – 12 d for direct photolysis in aqueous media (Harris 1982);

$\text{Biodegradation }$ $t_{1/2} = 72$ – 240 h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

$\text{Biodegradation }$ $t_{1/2} = 288$ – 960 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$\text{Biotransformation:}$

$\text{Bioconcentration, Uptake (k$_{1}$) and Elimination (k$_{2}$) Rate Constants:}$

$\text{Biota:}$
TABLE 16.1.7.7.1
Reported aqueous solubilities and vapor pressures of quinoline at various temperatures and the coefficients for the vapor pressure equations:

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure</th>
<th>Aqueous Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Summary of Literate Data</td>
<td>Van De Rostyne &amp; Prausnitz</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>59.7</td>
<td>133.3</td>
<td>12.62</td>
</tr>
<tr>
<td>89.6</td>
<td>666.6</td>
<td>16.71</td>
</tr>
<tr>
<td>103.8</td>
<td>1333</td>
<td>21.35</td>
</tr>
<tr>
<td>119.8</td>
<td>2666</td>
<td>22.42</td>
</tr>
<tr>
<td>136.7</td>
<td>5333</td>
<td>25.16</td>
</tr>
<tr>
<td>148.1</td>
<td>7999</td>
<td>28.25</td>
</tr>
<tr>
<td>163.2</td>
<td>13332</td>
<td>29.10</td>
</tr>
<tr>
<td>186.2</td>
<td>26664</td>
<td>35.90</td>
</tr>
<tr>
<td>212.3</td>
<td>53329</td>
<td>A 14.496</td>
</tr>
<tr>
<td>237.7</td>
<td>101325</td>
<td>B 4390.0</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–15.0</td>
<td>C 65.19</td>
</tr>
</tbody>
</table>

FIGURE 16.1.7.7.1 Logarithm of vapor pressure versus reciprocal temperature for quinoline.
### 16.1.7.8 Isoquinoline

- **Common Name:** Isoquinoline
- **Synonym:** Leucoline
- **Chemical Name:** Isoquinoline
- **CAS Registry No:** 119-65-3
- **Molecular Formula:** C<sub>9</sub>H<sub>7</sub>N
- **Molecular Weight:** 129.159
- **Melting Point (°C):** 26.47 (Lide 2003)
- **Boiling Point (°C):** 243.22 (Lide 2003)
- **Density (g/cm<sup>3</sup> at 20°C):**
  - 1.0986 (Weast 1982–83)
  - 1.0910 (Dean 1985)
- **Molar Volume (cm<sup>3</sup>/mol):**
  - 118.4 (30°C, Stephenson & Malanowski 1987)
  - 144.7 (calculated-Le Bas method at normal boiling point)
- **Dissociation Constant, pK:**
  - 5.40 (pK<sub>a</sub>, Perrin 1972)
  - 5.42 (pK<sub>a</sub>, 20°C, Weast 1982–83)
  - 5.40 (pK<sub>a</sub>, protonated cation + 1, Dean 1985)
  - 5.38 (pK<sub>a</sub>, protonated cation + 1, Riddick et al. 1986)
  - 5.39 (pK<sub>a</sub>, Sangster 1989)
- **Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):** 48.96 (bp, Riddick et al. 1986)
- **Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):** 7.448 (Riddick et al. 1986)
- **Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):**
- **Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F:** 0.967 (mp at 26.47°C)
- **Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):**
  - 4520 (Pearlman et al. 1984)

**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):**

- **11.8* (extrapolated-regression of tabulated data, temp range 63.5–240.5°C, Stull 1947)**
- **7.80 (extrapolated-Cox eq., Chao et al. 1983)**
  \[
  \log (P/\text{atm}) = [1− 516.182/(T/K)] \times 10^4(0.91210 – 6.33889 \times 10^{-4} \pm (T/K) + 4.267359 \times 10^{-7} \pm (T/K)^2]; \text{ temp range: 300.0–800.0 K (Cox eq., Chao et al. 1983)}
  \]
- **6.33 (extrapolated-Antoine eq., Boublik et al. 1984)**
  \[
  \log (P/\text{kPa}) = 6.03709 – 1723.459/(184.268 + t/°C); \text{ temp range 166–244°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
  \]
- **6.35 (extrapolated-Antoine eq., Dean 1985, 1992)**
  \[
  \log (P/\text{mmHg}) = 6.9122 – 1723.4/(184.3 + t/°C); \text{ temp range 167–244°C (Antoine eq., Dean 1992)}
  \]
- **6.70 (Riddick et al. 1986)**
  \[
  \log (P/\text{kPa}) = 6.03203 – 1719.5/(-89.12 + T/K); \text{ temp range 439–517 K (Antoine eq., Stephenson & Malanowski 1987)}
  \]
  \[
  \log (P/\text{mmHg}) = 45.5115 – 4.4715 \times 10^3/(T/K) – 13.308 \times 10^3/(T/K) + 4.0186 \times 10^{-3}(T/K) – 6.4589 \times 10^{-14}+(T/K)^2; \text{ temp range 299–803 K (vapor pressure eq., Yaws 1994)}
  \]
Henry’s Law Constant (Pa·m³/mol at 25°C):
19.14 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.08 (shake flask-UV, Hansch & Anderson 1967)
- 2.09 (HPLC-RT correlation, Mirrlees et al. 1976)
- 2.08 (recommended, Sangster 1989, 1993)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.30 ± 0.15, 2.17 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-$k'$ correlation, Cichna et al. 1995)
- 2.08 (recommended, Hansch et al. 1995)
- 2.21 ± 0.66, 2.2 6 ± 0.56 (HPLC-$k'$ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 3.09 (humic acid, HPLC-$k'$ correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{\frac{1}{2}}$:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 82.0$ h⁻¹, $k_2 = 34.2$ h⁻¹ ($daphnia pulex$, 21°C, Southworth et al. 1978)

Half-Lives in the Environment:
- Biota: elimination $t_{\frac{1}{2}} = 1$ min ($daphnia pulex$, Southworth et al. 1978).

<table>
<thead>
<tr>
<th>TABLE 16.1.7.8.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of isoquinoline at various temperatures</td>
</tr>
<tr>
<td>Stull 1947 summary of literature data</td>
</tr>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>63.5</td>
</tr>
<tr>
<td>92.7</td>
</tr>
<tr>
<td>107.8</td>
</tr>
<tr>
<td>123.7</td>
</tr>
<tr>
<td>141.6</td>
</tr>
<tr>
<td>152.0</td>
</tr>
<tr>
<td>167.6</td>
</tr>
<tr>
<td>190.0</td>
</tr>
<tr>
<td>214.5</td>
</tr>
<tr>
<td>240.5</td>
</tr>
</tbody>
</table>

mp/°C 24.5
FIGURE 16.1.7.8.1 Logarithm of vapor pressure versus reciprocal temperature for isoquinoline.
16.1.7.9 Benzo[f]quinoline

Common Name: Benzo[f]quinoline
Synonym: 5,6-benzoquinoline, naphthopyridine
Chemical Name: 5,6-benzoquinoline, benzo(f)quinoline
CAS Registry No: 85-02-9
Molecular Formula: C_{13}H_{9}N
Molecular Weight: 179.217
Melting Point (°C):
94 (Lide 2003)
Boiling Point (°C):
352 (Lide 2003)
Density (g/cm³ at 20°C):
196.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.15 (Sangster 1993)
Enthalpy of Fusion, Δ_{H_{ fus}} (kJ/mol):
Entropy of Fusion, Δ_{S_{ fus}} (J/mol K):
Fugacity Ratio at 25°C (assuming Δ_{S_{ fus}} = 56 J/mol K), F: 0.210 (mp at 94°C)
Water Solubility (g/m³ or mg/L at 25°C):
76.1 (shake flask-GC, Smith et al. 1978)
77.1 (Mill et al. 1981)
176.0 (Steen & Karickhoff 1981)
78.7 (average literature value, Pearlman et al. 1984)
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):
0.00747* (25.05°C, gas saturation, measured range 288.26–323.15 K, McEachern et al. 1975)
log (P/mmHg) = 4339.977/(T/K) + 10.2555; temp range 288.26–323.15 K (Antoine eq., gas saturation, McEachern et al. 1975)
0.00670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/L/kPa) = 9.37682 – 4338.411/(T/K); temp range 288–323 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0096 (calculated-P/C, Smith & Bomberger 1980)
Octanol/Water Partition Coefficient, log K_{ow}:
3.20 (Steen & Karickhoff 1981)
3.40 (TLC-RT correlation, De Voogt et al. 1988)
3.25 (23°C, shake flask-HPLC, pH 7, De Voogt et al. 1990)
3.25, 3.40 (lit. values; Sangster 1993)
3.46 ± 0.64, 3.51 ± 0.53 (HPLC-k’ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
2.18 (mixed microbial populations, Steen & Karickhoff 1981)
Sorption Partition Coefficient, log $K_{OC}$:

- 3.11 (Coyote Creek sediment, Smith et al. 1978)
- 4.64, 4.32 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 4.07 (humic acid, HPLC-$k'$ correlation, Nielsen et al. 1997)

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

Volatilization: estimated $t_\frac{1}{2} > 10000$ h in river, $t_\frac{1}{2} > 100000$ h in eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$$k = (1.4 \pm 0.7) \times 10^{-4} \text{ s}^{-1}$$
for transformation and transport when exposed to 12 h sunlight in mid-June with estimated $t_\frac{1}{2} = 2.8$ h in river, $t_\frac{1}{2} = 7.0$ h in eutrophic pond and eutrophic lake and $t_\frac{1}{2} = 1.4$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

$$t_\frac{1}{2} = 0.52 \text{ h in aquatics (Haque et al. 1980)}$$
$$t_\frac{1}{2} = 1 \text{ h for disappearance via direct photolysis in aqueous media (Harris 1982)}$$

Oxidation:

Laboratory studied $k < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with the $RO_2$ radicals and estimated $t_\frac{1}{2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$$k(\text{aq.}) = 3.7 \times 10^{-4} \text{ s}^{-1}$$
with $t_\frac{1}{2} = 0.5$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; $k(\text{aq.}) < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ with $t_\frac{1}{2} > 8 \text{ yr for free-radical oxidation in air-saturated water (NRCC 1983)}$

Hydrolysis:

Biodegradation: estimated $t_\frac{1}{2} = 190$ h in river, eutrophic pond, eutrophic lake and $t_\frac{1}{2} > 10^6$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_\frac{1}{2} = 0.5$ h in river water, $t_\frac{1}{2} = 6.9$ h in pond water, $t_\frac{1}{2} = 7.0$ h in eutrophic lake and $t_\frac{1}{2} = 1.4$ h in oligotrophic lake predicted by one-compartment for all processes including dilution (Smith et al. 1978)

$T_\frac{1}{2} = 1 \text{ h for disappearance via direct photolysis in aqueous media (Harris 1982)}$

**TABLE 16.1.7.9.1**

*Reported vapor pressures of benzo[f]quinoline at various temperatures*

<table>
<thead>
<tr>
<th>McEachern et al. 1975</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K</td>
</tr>
<tr>
<td>288.26</td>
</tr>
<tr>
<td>293.10</td>
</tr>
<tr>
<td>298.20</td>
</tr>
<tr>
<td>303.13</td>
</tr>
<tr>
<td>308.23</td>
</tr>
<tr>
<td>313.17</td>
</tr>
<tr>
<td>318.24</td>
</tr>
<tr>
<td>323.15</td>
</tr>
</tbody>
</table>

P/mmHg

$\log P = A - B/(T/K)$

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.2555</td>
<td>4399.977</td>
</tr>
</tbody>
</table>

$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 83.094$

$\Delta S_{\text{subl}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 196.36$
FIGURE 16.1.7.9.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[f]quinoline.
16.1.7.10 Carbazole

Common Name: Carbazole
Synonym: 9H-carbazole, dibenzopyrrole
Chemical Name: carbazole
CAS Registry No: 86-74-8
Molecular Formula: C_{12}H_{9}N, C_{6}H_{4}NHC_{6}H_{4}
Molecular Weight: 167.206
Melting Point (°C): 246.3 (Lide 2003)
Boiling Point (°C): 354.69 (Lide 2003)
Density (g/cm³ at 20°C): 1.260 (25°C, Jiménez et al. 1990)
Molar Volume (cm³/mol): 192.9 (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: 0.00674 (mp at 246.3°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.03 ± 0.05 (20°C, shake flask-GC, Smith et al. 1978)
1.037 (Mill et al. 1981)
0.428 (20°C, shake flask-fluorophotometry, Hashimoto et al. 1982)
1.67, 1.03, 0.908; 1.204 (quoted values; lit. average, Pearlman et al. 1984)
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):
7999* (248.2°C, summary of literature data, temp range: 248.2–354.8°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 15421.6/(T/K)] + 8.251923; temp range: 248.2–354.8°C (Antoine eq., Weast 1972–73)
0.0933 (20°C, Smith et al. 1978)
log (P/atm) = [1 – 627.897/(T/K)] × 10^{0.924810 – 5.18974 × 10–4 ± (T/K) + 2.68415 × 10–7 ± (T/K)^2}; temp range: 518.0–631.0 K (Cox eq., Chao et al. 1983)
0.00424 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.20101 – 2169.73/(162.465 + t°C); temp range 252.6–357.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 7.0863 – 2179.4/(163.5 + t°C); temp range 253–368°C (Antoine eq., Dean 1985, 1992)
0.0012 (Antoine eq.-I, Stephenson & Malanowski 1987)
0.0045 (liquid, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 10.1069 – 4780/(T/K); temp range not specified (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.21123 – 2179.424/(–109.636 + T/K); temp range 525–631 K (liquid, Antoine eq-II., Stephenson & Malanowski 1987)
log (P/mmHg) = 119.857 – 3.2537 × 10^{3}/(T/K) + 52.568-log (T/K) – 4.6797 × 10^{–2}–(T/K) + 1.4113 × 10^{–3}–(T/K)^2; temp range 518–899 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
16.0 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log $K_{ow}$:
3.29 (shake flask-UV at pH 7.4, Rogers 1969)
3.01 (HPLC-$k^′$ correlation, Eadsforth 1986)
3.50 (calculated, Eadsforth 1986)
3.72 (recommended, Sangster 1989, 1993)
3.59 (HPLC-RT correlation, Jenke et al. 1990)
3.84 (shake flask-HPLC at pH 7, De Voogt et al. 1988)
3.47 ± 0.63, 3.22 ± 0.53 (HPLC-$k^′$ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
3.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{sc}$:
2.24 (Coyote Creek sediment, Smith et al. 1978)
4.74 (humic acid, HPLC-$k^′$ correlation, Nielsen et al. 1997)
3.80 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:
Volatilization: estimated $t_\frac{1}{2}$ > 10⁵ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:
$k = 6.6 \times 10^{-5}$ s⁻¹ for transformation and transport when exposed to midday sunlight in late January with estimated $t_\frac{1}{2}$ = 6.0 h in river, $t_\frac{1}{2}$ = 15.0 h in eutrophic pond and eutrophic lake and $t_\frac{1}{2}$ = 3.0 h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)
photolytic $t_\frac{1}{2}$ = 1.0 h in aquatics (Haque et al. 1980)
$t_\frac{1}{2}$ = 3 h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation:
laboratory investigated $k = 29$ M⁻¹ s⁻¹ for the reaction with RO₂ radicals and estimated $t_\frac{1}{2}$ > 240 h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
$k(aq.) = 1.9 \times 10^{-4}$ s⁻¹ with $t_\frac{1}{2}$ = 1.0 h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; $k(aq.) = 29$ M⁻¹ s⁻¹ with $t_\frac{1}{2}$ = 280 yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-lives of 14 h in river, eutrophic pond, eutrophic lake and > 10³ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:
Surface water: estimated $t_\frac{1}{2}$ = 6.0 h in river, $t_\frac{1}{2}$ = 15.0 h in eutrophic pond and eutrophic lake and $t_\frac{1}{2}$ = 3.0 h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978);
photolytic $t_\frac{1}{2}$ = 1.0 h in aquatics (Haque et al. 1980); $t_\frac{1}{2}$ = 3 h for disappearance via direct photolysis in aquatic media (Harris 1982).
TABLE 16.1.7.10.1
Reported vapor pressures of carbazole at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

**Stull 1947**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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</thead>
<tbody>
<tr>
<td>248.2</td>
<td>7999</td>
<td>73.43</td>
<td>0.0610</td>
</tr>
<tr>
<td>265.0</td>
<td>13332</td>
<td>78.72</td>
<td>0.101</td>
</tr>
<tr>
<td>292.5</td>
<td>26664</td>
<td>81.0</td>
<td>0.129</td>
</tr>
<tr>
<td>323.0</td>
<td>53329</td>
<td>83.59</td>
<td>0.167</td>
</tr>
<tr>
<td>354.8</td>
<td>101325</td>
<td>86.67</td>
<td>0.219</td>
</tr>
<tr>
<td>87.13</td>
<td>0.227</td>
<td></td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>244.8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90.80</td>
<td>0.329</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

ρ (at 25°C) 1.26 g/cm³

eq. 1 P/Pa

A 14.04

B 5288.4

enthalpy of sublimation:

\[\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 103.3\]

at 25°C

**Jiménez et al. 1990**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>73.43</td>
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<tr>
<td>78.72</td>
<td>0.101</td>
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<tr>
<td>81.0</td>
<td>0.129</td>
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<td>83.59</td>
<td>0.167</td>
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<td>86.67</td>
<td>0.219</td>
</tr>
<tr>
<td>87.13</td>
<td>0.227</td>
</tr>
<tr>
<td>90.80</td>
<td>0.329</td>
</tr>
</tbody>
</table>

FIGURE 16.1.7.10.1 Logarithm of vapor pressure versus reciprocal temperature for carbazole.
16.1.7.11 Benzo[c,g]carbazole

Common Name: Benzo[c,g]carbazole
Synonym: 7H-dibenzo[c,g]carbazole
Chemical Name: 7H-dibenzo[c,g]carbazole
CAS Registry No: 194-59-2
Molecular Formula: C$_{20}$H$_{13}$N, C$_{10}$H$_6$NHC$_{10}$H$_6$
Molecular Weight: 267.324
Melting Point (°C):
  158 (Lide 2003)
Boiling Point (°C)
Density (g/cm$^3$ at 20°C):
Molar Volume (cm$^3$/mol):
  296.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK$_a$:
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: 0.0496 (mp at 158°C)
Water Solubility (g/m$^3$ or mg/L at 25°C):
  0.063 ± 0.003 (shake flask-GC, Smith et al. 1978)
  0.064 (Mill et al. 1981)
  0.064 (Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C):
  $1.33 \times 10^{-7}$ (estimated by comparison with benzo[a]pyrene, Smith et al. 1978)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
  0.00048 (calculated-P/C, Smith & Bomberger 1980)
Octanol/Water Partition Coefficient, log K$_{OW}$:
5.75 (calculated-S, Steen & Karickhoff 1981)
Octanol/Air Partition Coefficient, log K$_{OA}$:
Bioconcentration Factor, log BCF:
  4.93 (mixed microbial populations, Steen & Karickhoff 1981)
Sorption Partition Coefficient, log K$_{OC}$:
  4.31 (Coyote Creek sediment, Smith et al. 1978)
  6.03, 6.16 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
Environmental Fate Rate Constants, k, or Half-Lives, $t_\text{½}$:
Volatilization: estimated $t_\text{½}$ = 15000 h in river, $t_\text{½}$ = 37000 h in eutrophic pond, $t_\text{½}$ = 73000 h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).
Photolysis: rate constant
  $k = 5.2 \times 10^{-4}$ s$^{-1}$ for transformation and transport when exposed to midday sunlight in mid-January with estimated $t_\text{½}$ = 1.0 h in river, $t_\text{½}$ = 1.5 h in eutrophic pond and eutrophic lake and $t_\text{½}$ = 0.5 h in oligotrophic lake assuming winter insulation by the one compartment model (Smith et al. 1978)
  photolytic $t_\text{½}$ = 0.35 h in aquatics (Haque et al. 1980).
Nitrogen and Sulfur Compounds

Oxidation:
laboratory studied $k = 830 \text{ M}^{-1} \text{s}^{-1}$ for the reaction with the $\text{RO}_{2}$ radicals and estimated $t_{1/2} > 700 \text{ h}$ in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k = 5.5 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ under natural sunlight conditions for midday, midsummer at a latitude of $40^\circ \text{N}$; $k = 830 \text{ M}^{-1} \text{s}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:
Biodegradation: estimated half-life to be very long in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model with no acclimated cultures obtained during the screening studies (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:
Surface water: $t_{1/2} = 0.36 \text{ h}$ in river water, $t_{1/2} = 1.5 \text{ h}$ in pond water, $t_{1/2} = 1.5 \text{ h}$ in eutrophic lake and $t_{1/2} = 0.5 \text{ h}$ in oligotrophic lake for all processes predicted by one-compartment model (Smith et al. 1981);
$t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturated water (NRCC 1983).
16.1.7.12 Acridine

Common Name: Acridine
Synonym: 2,3,5,6-dibenzopyridine
Chemical Name: acridine, 2,3,5,6-dibenzopyridine
CAS Registry No: 260-94-6
Molecular Formula: C_{13}H_9N
Molecular Weight: 179.217
Melting Point (°C):
110  (Lide 2003)
Boiling Point (°C):
344.86  (Lide 2003)
Density (g/cm³ at 20°C):
1.005  (Weast 1982–83)
Molar Volume (cm³/mol):
196.3  (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
5.60  (Albert 1966; Matzner et al. 1991; Matzner & Bales 1994)
5.58  (20°C, Weast 1982–83)
5.60  (protonated cation + 1, Dean 1985)
10.65  (Sangster 1989)
Enthalpy of Fusion, ΔHₕₕ (kJ/mol):
18.58 ± 0.38  (McEachern et al. 1975)
Entropy of Fusion, ΔSₕₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕₕ = 56 J/mol K), F: 0.147 (mp at 110°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
57.4  (Albert 1966)
38.4  (24°C, shake flask-LSC, Means et al. 1980)
46.6  (literature average, Pearlman et al. 1984)
54.8  (centrifuge-HPLC at pH 8, Matzner et al. 1991)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designed * are compiled at the end of this section):
133.3*  (129.4°C, summary of literature data, temp range 129.4–346°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 15174.6/(T/K)] + 8.251980; temp range 129.4–346°C (Antoine eq., Weast 1972–73)
0.0065*  (Langmuir free evaporation, measured range 7.96–50°C, McEachern et al. 1975)
log (P/mmHg) = 27.076 – 11021.64/(T/K); measured range 281.2–323.3 K (Langmuir free evaporation, McEachern et al. 1975)
0.0075  (extrapolated-Cox eq., Chao et al. 1983)
log (P/atm) = [1 – 618.827/(T/K)] × 10^{0.839996 – 4.19344 × 10^{-4} ± (T/K) + 3.63487 × 10^{-7} ±(T/K)^2}; temp range: 402.6–619.2 K (Cox eq., Chao et al. 1983)
0.2066  (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1983)
0.0065  (Interpolated-Antoine eq.-I, Stephenson & Malanowski 1987; quoted, Ma et al. 1990)
Nitrogen and Sulfur Compounds

log (P_s/kPa) = 8.30838 – 3365.943/(-48.723 + T/K); temp range 293–367 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_l/kPa) = 6.73664 – 2699.39/(-48.611 + T/K); temp range 402–619 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m^3/mol at 25°C):

0.030 (calculated-P/C, Ma et al. 1990)

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

3.40 (shake flask-UV, Hansch & Fujita 1964)
3.39 (HPLC-RT correlation, Mirrlees et al. 1976)
3.39 (shake flask at pH 7.4, Unger et al. 1978)
3.62 (shake flask-LSC, Means et al. 1980)
3.29 (shake flask-AS at pH 7.4, Unger & Chiang 1981)
3.31 ± 0.03 (HPLC-RV correlation-ALPM, Garst 1984)
3.35 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
3.32 (shake flask-GC at pH 7.0, Haky & Leja 1986)
3.40 (recommended, Sangster 1989, 1993)
3.40 (recommended, Hansch et al. 1995)
3.18 ± 0.64, 3.27 ± 0.53 (HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

2.40 (selected, Ma et al. 1990)

Bioconcentration Factor, log BCF:

2.40 (selected, Ma et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

4.69 (average of sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
3.32 (calculated, Means et al. 1980)
-0.157 (estimated of Loring subsurface material, Zachara et al. 1987)
0.610 (estimated of Anvil Points subsurface material, Zachara et al. 1987)
3.09–3.41 (soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987)
3.16–3.33 (soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987)
2.36–2.52 (soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987)
2.98–3.30 (soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987)
2.19–2.48 (soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987)
4.22, 4.26 (soil, quoted, calculated-MCI χ, Sabljic 1987)
4.11, 3.32 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
4.11, 4.31 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.00 (HPLC-k′ correlation, Nielsen et al. 1997)
4.79 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:

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

k_1 = 109 h^{-1}, k_2 = 3.68 h^{-1} (daphnia pulex, 21°C, Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination t_1/2 = 11.3 min (daphnia pulex, Southworth et al. 1978).
TABLE 16.1.7.12.1
Reported vapor pressures of acridine at various temperatures and the coefficients for the vapor pressure equations

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

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<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>25.05</td>
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<tr>
<td>25.05</td>
<td>0.00656</td>
<td>40.02</td>
<td>0.0380</td>
<td>50.0</td>
<td>0.1074</td>
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Stull 1947

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<tr>
<td>129.4</td>
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<td>284.0</td>
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McEachern et al. 1975

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<td>25.05</td>
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<td>11021.64</td>
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<td>temp range: 281.2–323.2 K</td>
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<td>enthalpy of fusion: 18.58 kJ mol⁻¹</td>
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<td>enthalpy of vaporization: 72.59 kJ mol⁻¹</td>
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</tr>
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<td>121.75</td>
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<td>72.59</td>
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</tbody>
</table>

FIGURE 16.1.7.12.1 Logarithm of vapor pressure versus reciprocal temperature for acridine.
16.1.8 SULFUR COMPOUNDS

16.1.8.1 Carbon disulfide

\[
\text{S} = \text{C} = \text{S}
\]

Common Name: Carbon disulfide
Synonym: carbon disulphide
Chemical Name: carbon disulfide
CAS Registry No: 75-15-0
Molecular Formula: CS₂
Molecular Weight: 76.141
Melting Point (°C):
-112.1 (Lide 2003)
Boiling Point (°C):
46 (Lide 2003)
Density (g/cm³):
1.2632 (20°C, Weast 19820–83)
1.26311, 1.2555 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
66.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
27.522, 26.736 (25°C, bp, Riddick et al. 1986)
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
4.389 (Riddick et al. 1986)
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
2100 (20°C, selected, 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):

53329* (28°C, summary of literature data, temp range –73.8 to 46.5°C, Stull 1947)
47359* (24.582°C, comparative ebulliometry, measured range 3.6–80°C, Waddington et al. 1962)
\[
\log (P/\text{mmHg}) = 6.94194 - 1168.623/(241.534 + t/°C); \text{ temp range 3.6–80°C (Antoine eq., comparative ebulliometry, Waddington et al. 1962)}
\]
\[
\log (P/\text{kPa}) = 6.86752 - 1169.022/(241.582 + t/°C), \text{ temp range 3.6–80°C (Antoine eq. derived from exp. data of Waddington et al. 1949, Boublik et al. 1984)}
\]
\[
\log (P/\text{kPa}) = 6.03385 - 1151.908/(239.748 + t/°C), \text{ temp range –17.76 to 45.14°C (Antoine eq. derived from exp. data, Boublik et al. 1984)}
\]
48210 (selected, Riddick et al. 1986)
\[
\log (P/\text{kPa}) = 6.06694 - 1168.623/(t/°C + 241.534) \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]
\[
\log (P_f/\text{kPa}) = 6.03694 - 1153.5((-33.22 + T/K); \text{ temp range 256–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P_f/\text{kPa}) = 6.07588 - 1174.112/(-30.896 + T/K); \text{ temp range 260–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P_f/\text{kPa}) = 6.1914 – 1231.307/(-26.024 + T/K); \text{ temp range 338–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P_f/\text{kPa}) = 6.80466 – 1278.903/(43.404 + T/K); \text{ temp range 388–497 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]
\[
\log (P_f/\text{kPa}) = 7.58592 – 2639.181/(165.312 + T/K); \text{ temp range 490–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]

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log (P/mmHg) = 25.1475 – 2.0349 × 10³/(T/K) – 6.7794·log (T/K) + 3.4828 × 10⁻³·(T/K) – 1.0105 × 10⁻¹⁴·(T/K)²;

temp range 162–552 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
142 (calculated-P/C, Howard 1990)
1946 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1577 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log Kₐw = 3.485 – 1077/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kₒw:
1.70–4.60 (Hansch & Leo 1985)
2.14 (recommended, Sangster 1993)
1.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₒa:

Bioconcentration Factor, log BCF or log K₉:
0.90 (calculated-solubility, Howard 1990)

Sorption Partition Coefficient, log Kₒc:
1.80 (calculated-solubility, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization: t½ = 2.6 h in a model river (Howard 1990)
Photolysis:
Oxidation:
Hydrolysis: t½ = 1.1 yr at pH 9 in alkaline solution (Howard 1990)
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):

Half-Lives in the Environment:
Air: t½ = 9 d degraded by reacting with atomic oxygen and photochemically produced OH radicals (Howard 1990)

**TABLE 16.1.8.1.1**
Reported vapor pressures of carbon disulfide at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>log P = A – B/(T/K)</th>
<th>ln P = A – B/(T/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>–73.8</td>
<td>133.3</td>
<td>3.588</td>
<td>19920</td>
</tr>
<tr>
<td>–54.3</td>
<td>666.6</td>
<td>8.772</td>
<td>25007</td>
</tr>
<tr>
<td>–44.7</td>
<td>1333</td>
<td>13.999</td>
<td>31168</td>
</tr>
<tr>
<td>–34.3</td>
<td>2666</td>
<td>19.269</td>
<td>38547</td>
</tr>
<tr>
<td>–22.5</td>
<td>5333</td>
<td>24.582</td>
<td>47359</td>
</tr>
<tr>
<td>–15.3</td>
<td>7999</td>
<td>29.927</td>
<td>57803</td>
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</table>

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### TABLE 16.1.8.1.1 (Continued)

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Waddington et al. 1962</th>
<th>Boublík &amp; Aim 1972</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>–5.1</td>
<td>13332</td>
<td></td>
</tr>
<tr>
<td>10.4</td>
<td>26664</td>
<td></td>
</tr>
<tr>
<td>28.0</td>
<td>53329</td>
<td></td>
</tr>
<tr>
<td>46.5</td>
<td>101325</td>
<td>57.295</td>
</tr>
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<td></td>
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<td>68.531</td>
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<td>79.927</td>
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</table>

<table>
<thead>
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<th>Carbon disulfide: vapor pressure vs. 1/T</th>
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</thead>
<tbody>
<tr>
<td><img src="image.png" alt="Graph" /></td>
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</tbody>
</table>

**FIGURE 16.1.8.1.1** Logarithm of vapor pressure versus reciprocal temperature for carbon disulfide.
16.1.8.2 Dimethyl sulfide

Common Name: Dimethyl sulfide
Synonym: DMS, methyl sulfide, thiobismethane, 2-thiopropane
Chemical Name: dimethyl sulfide
CAS Registry No: 75-18-3
Molecular Formula: C₂H₆S, (CH₃)₂S
Molecular Weight: 62.134
Melting Point (°C):
-98.24 (Lide 2003)
Boiling Point (°C):
37.33 (Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 25°C):
0.84825, 0.84230 (20°C, 25°C, Dreisbach 1961)
0.8423 (Riddick et al. 1986)
Molar Volume (cm³/mol):
73.2 (Kamlet et al. 1986)
73.8 (20°C, calculated-density)
77.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK₆:
-6.99 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
27.49, 26.82 (25°C, bp, Dreisbach 1961)
27.65, 27.0 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH₉ (kJ/mol):
7.99 (Riddick et al. 1986)
Entropy of Fusion, ΔS₉ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
15606 (Hine & Mookerjee 1975)
6300 (Verschueren 1983)
22000 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)
20000 (Riddick et al. 1986)
19600 (selected, Yaws et al. 1990)
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):
53174* (20.087°C, static method, measured range −22.547 to 20.087°C, Osborn et al. 1942)
log (P/mmHg) = 16.51798 − 1876.370/(T/K) − 3.04727 ± log (T/K); temp range −22.547 to 20.087°C (static method, Osborn et al. 1942)
53329* (18.7°C, summary of literature data, temp range −75.6 to 36°C, Stull 1947)
64650 (calculated from determined data, Dreisbach 1961)
log (P/mmHg) = 6.93138 − 1081.587/(229.746 + t/°C), temp range −50 to 130°C (Antoine eq. for liquid state, Dreisbach 1961)
64501* (interpolated-Antoine eq., temp range −47.4 to 58.319°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.94879 − 1090.755/(230.799 + t/°C); temp range −47.4 to 58.319°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
70300 (Hine & Mookerjee 1975)
log (P/mmHg) = [−0.2185 × 6742.3/(T/K)] + 7.589204; temp range −75 to 224.5°C (Antoine eq., Weast 1972–73)
56000 (20°C, Verschueren 1983)
64443 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
64460 (extrapolated-Antoine eq., Boublik et al. 1984)
log \( (P/kPa) = 6.27843 - 1196.875/(242.81 + t/°C) \), temp range –22.55 to 20.09°C ( Antoine eq. from reported expitl. data, Boublík et al. 1984)

64470 (extrapolated-Antoine eq., Dean 1985, 1992)

log \( (P/mmHg) = 7.1509 - 1195.58/(242.68 + t/°C) \); temp range –22 to 20°C ( Antoine eq., Dean 1985, 1992)

64650 (quoted, Riddick et al. 1986)

log \( (P/kPa) = 6.07369 - 1090.755/(230.799 + t/°C) \); temp range not specified ( Antoine eq., Riddick et al. 1986)

64520 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

log \( (P/kPa) = 6.07043 - 1088.851/(–42.594 + T/K) \); temp range 268–319 K ( Antoine eq.-I, Stephenson & Malanowski 1987)

log \( (P/kPa) = 6.13042 - 1124.998/(–37.961 + T/K) \); temp range 307–379 K ( Antoine eq.-II, Stephenson & Malanowski 1987)

log \( (P/kPa) = 6.42655 - 1344.329/(–7.456 + T/K) \); temp range 372–453 K ( Antoine eq.-III, Stephenson & Malanowski 1987)

log \( (P/kPa) = 7.36327 - 2293.043/(130.243 + T/K) \); temp range 372–453 K ( Antoine eq.-IV, Stephenson & Malanowski 1987)

log \( (P/mmHg) = 37.2604 – 2.4251 \times 10^3/(T/K) – 11.384·\log (T/K) + 5.8122 \times 10^{-3}·(T/K) + 8.5893 \times 10^{-14}·(T/K)^2 \); temp range 175–503 K (vapor pressure eq., Yaws 1994)

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

278.1 \((1/K_{AW, exptl.}, Hine & Mookerjee 1975)\)

298, 366.6 \((\text{calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975})\)

165 \((20°C, \text{headspace-GC, Vitenberg et al. 1975})\)

180.4, 184.7, 173.5 \((\text{headspace-GC, concn. of 10, 1.0, 0.1 ppm by weight, Przyjazny et al. 1983})\)

180.4, 184.7, 173.5 \((\text{headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983})\)

log \( (1/K_{AW}) = 1637.3/(T/K) – 4.354; \text{temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983})\)

log \( (1/K_{AW}) = 1635.6/(T/K) – 4.358; \text{temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983})\)

log \( (1/K_{AW}) = 1598.2/(T/K) – 4.205; \text{temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983})\)

163.4 \((\text{quoted, Gaffney et al. 1987})\)

184, 1271 \((\text{quoted, calculated-molecular structure, Russell et al. 1992})\)

138 \((20°C, \text{selected from literature experimentally measured data, Staudinger & Roberts 1996})\)

233.0* \((\text{equilibrium headspace-GC, in seawater, measured range 18–44°C, Wong & Wang 1997})\)

61.97 \((\text{equilibrium headspace-GC, Marin et al. 1999})\)

155 \((20°C, \text{selected from literature experimentally measured data, Staudinger & Roberts 2001})\)

log \( K_{AW} = 3.556 – 1394/(T/K) \), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( K_{OW} \):

Octanol/Air Partition Coefficient, \( K_{OA} \):

Bioconcentration Factor, \( BCF \):

Sorption Partition Coefficient, \( K_{OC} \):

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

Volatilization:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$k_{\text{OH}}^* = (9.80 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.9 K, measured range 299.9–426.5 K (flash photolysis-resonance fluorescence, Atkinson et al. 1978)

$k_{\text{OH}}^* = (8.28 \pm 0.87) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 273–400 K by flash photolysis-resonance fluorescence, Kurylo 1978)

$k_{\text{O(3P)}}^* = \frac{57 \times 10^{-12}}{} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with O(3P) atom at 296 K, measured range 252–493 K (Sagle et al. 1978)

$k_{\text{OH}}^* = (4.26 \pm 0.56) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 248–363 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

$k_{\text{OH}} = (1.0 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated lifetime $\tau \sim 30$ h in the daytime,

$k_{\text{O(3P)}} = (5.4 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated $\tau \sim 3$ h in the nighttime hours at 296 ± 2 K (Atkinson et al. 1984)

$k_{\text{O3}} < 8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.05 \text{ d}^{-1}$, $k_{\text{OH}} = 9.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d$^{-1}$, and $k_{\text{NO3}} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d$^{-1}$ at room temp. (review, Atkinson & Carter 1984)

$k_{\text{O3}} < 8 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 6.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.27 d$^{-1}$, and $k_{\text{NO3}} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d$^{-1}$ at room temp. (review, Atkinson 1985)

$k_{\text{OH}}^* = (4.09, 4.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 267–397 K (flash photolysis-resonance fluorescence, Hynes et al. 1986)

$k_{\text{OH}}^* = (3.60 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–440 K by flash photolysis-resonance fluorescence; $k_{\text{OH}} = 9.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to $n$-hexane, $k_{\text{OH}} = 5.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to cyclohexane at 296 K (Wallington et al. 1986a)

$k_{\text{NO3}}^* = (8.1 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 280–350 K (flash photolysis-visible absorption, Wallington et al. 1986b)

$k_{\text{OH}}^* = (5.50 \pm 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 260–393 K (discharge flow-resonance fluorescence, Hsu et al. 1987)

$k_{\text{OH}} = (8.0 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Relative rate method, Barnes et al. 1989)

$k_{\text{OH}} = 3.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 3.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{NO3}}^* = (10.6 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 256–376 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{\text{OH}} = 4.56 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 4.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO3}} = 9.77 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO3}}^* = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime $\tau \sim 30$ h due to reaction with OH radical in the daytime and $\tau \sim 3$ h due to reaction at night with NO$_3$ radical (Atkinson et al. 1984); calculated lifetimes, $\tau > 20$ d due to reaction with O$_3$ in 24-h, $\tau = 28$ h with OH radical during daytime and $\tau = 120$ min with NO$_3$ radical during nighttime in “clean” atmosphere; $\tau > 3$ d due to reaction with O$_3$ in 24-h, $\tau = 420$ min with OH radical in daytime and $\tau = 13$ min with NO$_3$ in nighttime in “moderately polluted” atmosphere (Winer et al. 1984)

estimated tropospheric chemical lifetimes, $\tau = 2$ d, 2 d and > 15 d for reactions with OH, NO$_3$ and O$_3$, respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)
### TABLE 16.1.8.2.1
Reported vapor pressures and Henry's law constants of dimethyl sulfide at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Vapor pressure</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>static method-manometer</td>
<td>summary of literature data</td>
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<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
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<tr>
<td>-22.547</td>
<td>6994</td>
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<td>4.943</td>
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<td>15.138</td>
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<tr>
<td>20.087</td>
<td>53174</td>
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<tr>
<td>$mp/K$</td>
<td>174.855</td>
<td>2.60</td>
</tr>
<tr>
<td>$bp/K$</td>
<td>310.49</td>
<td>18.7</td>
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<td>log $P = A - B/(T/K) - C\cdot\log (T/K)$</td>
<td>8.883</td>
<td>33331</td>
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<tr>
<td>$A$</td>
<td>16.51798</td>
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<tr>
<td>$B$</td>
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<td>$C$</td>
<td>3.04727</td>
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<tr>
<td>$\Delta H_{fus}/(kJ mol^{-1}) = 7.985$</td>
<td>36.572</td>
<td>98659</td>
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<tr>
<td>$\Delta C_v/(kJ mol^{-1}) = 27.98$</td>
<td>25</td>
<td>64501</td>
</tr>
</tbody>
</table>

Antoine eq.

$\log P = A - B/(C + t/°C)$

$P/mmHg$

$A$ | 6.94879 |
$B$ | 1090.755 |
$C$ | 230.799 |

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

at 25$°C$ | 27.65 |
at $bp$ | 26.92 |
**FIGURE 16.1.8.2.1** Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfide.

**FIGURE 16.1.8.2.2** Logarithm of Henry's law constant versus reciprocal temperature for dimethyl sulfide.
16.1.8.3 Dimethyl disulfide

\( \text{S-S} \)

Common Name: Dimethyl disulfide
Synonym: 2,3-dithiabutane
Chemical Name: dimethyl didisulfide
CAS Registry No: 624-92-0
Molecular Formula: \( \text{C}_2\text{H}_6\text{S}_2, \text{ CH}_3\text{SSCH}_3 \)
Molecular Weight: 94.199
Melting Point (°C):
\(-84.67 \) (Lide 2003)
Boiling Point (°C):
109.74 (Lide 2003)
Density (g/cm³):
1.6025 (20°C, Weast 1982–83)
Dissociation Constant, \( \text{pK}_a \):
Molar Volume (cm³/mol):
103.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
38.37, 33.68 (25, bp, Zwolinski & Wilhoit 1971)
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), \( F: 1.0 \)
Water Solubility (g/m³ or mg/L at 25°C):
3400 (estimated-activity coefficient by headspace-GC, Przyjazny 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):
3825* (static method, measured range 0–60°C, Scott et al. 1950)
\( \log (P/\text{mmHg}) = 6.97792 – 1396.342/(218.863 + t/°C) \); temp range 5.356 –109.745°C (Antoine eq., Zwolinski & Wilhoit 1971)
3850 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
\( \log (P/\text{mmHg}) = 6.18000 – 1389.151/(223.184 + t/°C), \) temp range 0–60°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)
\( \log (P/\text{kPa}) = 6.08703 – 1336.665/(217.767 + t/°C), \) temp range 61.4–128.6°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)
\( \log (P/\text{mmHg}) = 9.9328-\log (T/K) + 2.2831 \times 10^{-11}(T/K) + 3.1730 \times 10^{-6}(T/K)^2; \) temp range 125–499 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
121 (20°C, headspace-GC, Vitenberg et al. 1975)
112, 101 (headspace-GC, concn. of 10 and 1.0 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
\( \log (1/K_{aw}) = 1657.1/(T/K) – 4.211; \) temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
\( \log (1/K_{aw}) = 1854.4/(T/K) – 4.828; \) temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
77.5 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
\[
\log K_{AW} = 4.828 - 1384/(T/K), \text{ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 1.77 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.77 (recommended, Sangster 1993)
- 1.77 (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, \( t_{1/2} \), or Lifetimes, \( \tau \):
- 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:
  - \( k_{OH} = 2.40 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), at 297 K (relative rate method, Cox & Sheppard 1980)
  - \( k_{OH}^* = (1.84 - 19.8) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), at 298 K, measured range 255–377 K (flask photolysis-resonance fluorescence, Wine et al. 1984)
  - \( k_{OH}^* = 2.05 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), at 298 K (tentative recommended, Atkinson 1985)
  - \( k_{NO3}^* = 4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K, measured range 280–350 K (flash photolysis-optical absorption, Wallington et al. 1986)
  - \( k_{NO3}^* = (7.3 \pm 1.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp., measured range 334–382 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)
  - \( k_{NO3} = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), independent of temperature over the range ~300–380 K (recommended, Atkinson 1991)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
  - Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:
### TABLE 16.1.8.3.1
Reported vapor pressures of dimethyl disulfide at various temperatures and the coefficients for the vapor pressure equations

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

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

(2) \quad \ln P = A - B/(C + t^\circ C) \quad (2a)

(3) \quad \text{selected values}

\[
\begin{array}{cccccc}
\text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} \\
0 & 904 & 61.411 & 19920 & 5.356 & 1333 \\
15 & 2230 & 67.301 & 25007 & 18.299 & 2666 \\
20 & 2936 & 73.234 & 31160 & 25.891 & 4000 \\
25 & 3825 & 79.201 & 38547 & 31.579 & 5333 \\
30 & 4930 & 85.218 & 47359 & 36.177 & 6666 \\
35 & 6301 & 91.283 & 57803 & 40.060 & 7999 \\
40 & 7975 & 97.393 & 70109 & 46.435 & 10666 \\
45 & 10007 & 103.542 & 84525 & 51.600 & 13332 \\
50 & 12448 & 109.738 & 101325 & 61.518 & 19998 \\
55 & 15359 & 115.984 & 120798 & 69.008 & 26664 \\
60 & 18813 & 122.273 & 143268 & 75.099 & 33331 \\
& & 128.611 & 169052 & &
\end{array}
\]

Scott et al. 1950

\[
\begin{array}{cccccc}
\text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} \\
0 & 904 & 61.411 & 19920 & 5.356 & 1333 \\
15 & 2230 & 67.301 & 25007 & 18.299 & 2666 \\
20 & 2936 & 73.234 & 31160 & 25.891 & 4000 \\
25 & 3825 & 79.201 & 38547 & 31.579 & 5333 \\
30 & 4930 & 85.218 & 47359 & 36.177 & 6666 \\
35 & 6301 & 91.283 & 57803 & 40.060 & 7999 \\
40 & 7975 & 97.393 & 70109 & 46.435 & 10666 \\
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50 & 12448 & 109.738 & 101325 & 61.518 & 19998 \\
55 & 15359 & 115.984 & 120798 & 69.008 & 26664 \\
60 & 18813 & 122.273 & 143268 & 75.099 & 33331 \\
& & 128.611 & 169052 & &
\end{array}
\]

Zwolinski & Wilhoit 1971

\[
\begin{array}{cccccc}
\text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{bp/°C} & \Delta H_v/(kJ mol^{-1}) \\
0 & 904 & 61.411 & 19920 & 5.356 & 1333 \\
15 & 2230 & 67.301 & 25007 & 18.299 & 2666 \\
20 & 2936 & 73.234 & 31160 & 25.891 & 4000 \\
25 & 3825 & 79.201 & 38547 & 31.579 & 5333 \\
30 & 4930 & 85.218 & 47359 & 36.177 & 6666 \\
35 & 6301 & 91.283 & 57803 & 40.060 & 7999 \\
40 & 7975 & 97.393 & 70109 & 46.435 & 10666 \\
45 & 10007 & 103.542 & 84525 & 51.600 & 13332 \\
50 & 12448 & 109.738 & 101325 & 61.518 & 19998 \\
55 & 15359 & 115.984 & 120798 & 69.008 & 26664 \\
60 & 18813 & 122.273 & 143268 & 75.099 & 33331 \\
& & 128.611 & 169052 & &
\end{array}
\]

\[
\begin{align*}
\text{Scott et al. 1950} & \quad \text{Zwolinski & Wilhoit 1971} \\
A &= 6.97792 & \quad A = 1396.342 \\
B &= 1396.342 & \quad B = 218.863 \\
C &= 218.863 & \quad C = 6.97792
\end{align*}
\]

\[
\Delta H_v/(kJ mol^{-1}) = 88.812 \quad \Delta H_v/(kJ mol^{-1}) = 95.780
\]

at 25°C \quad at bp

95.780 \quad 101.712

9.780 \quad 33.68

109.745 \quad 38.37

88.812 \quad 38.37

88.812 \quad 38.37

88.812 \quad 38.37

88.812 \quad 38.37

FIGURE 16.1.8.3.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl disulfide.
16.1.8.4 Dimethyl sulfoxide (DMSO)

Common Name: Dimethyl sulfoxide
Synonym: DMSO, sulfinylbismethane, methyl sulfoxide, methylsulfinylmethane, SQ 9453, DMS-70, DMS-90, Deltan, Demasorb, Demavet, Demeso, Dermasorb, Dolicur, Domoso, Dromisol, Gamasol 90, Hyadur, Rimso-50, Sclerosol, Somipront, Sotexan, Topsym
Chemical Name: dimethyl sulfoxide
CAS Registry No: 67-68-5
Molecular Formula: C₂H₆OS, (CH₃)₂SO
Molecular Weight: 78.133
Melting Point (°C): 17.89 (Lide 2003)
Boiling Point (°C): 189.0 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 25°C): 1.1014 (Weast 1982–83)
Molar Volume (cm³/mol): 85.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ: 1.4 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔHV (kJ/mol): 52.88, 43.14 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol): 14.368 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K): Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C): 253000 (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):
80.0* (gas saturation, measured range 20–50°C, Douglas 1948)
log (P/mmHg) = 26.49588 – 3539.32/(T/K) – 6.000 ± ln (T/K); temp range 20–50°C (gas saturation, Douglas 1948)
460* (52.35°C, Hg manometer, measured range 325.5–442.1 K, Jakli & van Hook 1972)
ln (P/mmHg) = 17.4922 – 4517.79/(T/K – 47.2583); temp range 291.7–463 K (Hg manometer, Antoine eq. with literature data, Jakli & van Hook 1972)
56.0 (20°C, Verschueren 1983)
80.9 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.64816 – 1922.32/(223.353 + t°C); temp range 52.4–168.95°C (Antoine eq. from reported exptl. data of Jakli & von Hook 1972, Boublik et al. 1984)
80.0 (selected, Riddick et al. 1986)
log (P/kPa) = 6.72161 – 1962.06/(225.892 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
79.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.72167 – 1962.05/(–47.258 + T/K); temp range 305–464 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 45.4653 – 4.0439 × 10⁻⁴(T/K) – 13.21 log (T/K) + 1.0981 × 10⁻⁲(T/K) + 6.4155 × 10⁻⁶(T/K)²; temp range 292–465 K (vapor pressure eq., Yaws et al. 1994)

Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log $K_{OW}$:
-1.35  (shake flask, Hansch & Leo 1979, 1987)
-0.85  (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
-1.35  (recommended, Sangster 1989)
-1.35  (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

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

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

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:
$k_{OH} = (6.2 \pm 2.2) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{NO3} = (1.7 \pm 0.3) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{O3} < 5.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp (Barnes et al. 1989)
$k_{OH} = (62 \pm 25) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (Atkinson 1989)
$k_{OH} = (1.0 \pm 0.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp (Hynes & Wine 1996)
$k_{OH} = (8.7 \pm 1.6) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Urbanski et al. 1998)
$k_{OH} = (5.9 \pm 1.5) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with tropospheric lifetime $\tau = 5$ h, $k_{NO3} = (5.0 \pm 3.8) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with tropospheric lifetime $\tau = 3$ d; $k_{O3} < 1.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with tropospheric lifetime $\tau > 150$ d and $k_{Cl} = (7.4 \pm 1.0) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with Cl atoms with tropospheric lifetime $\tau = 62$ d at room temp and 740 torr (Relative rate method, Falbe-Hansen et al. 2000)

Hydrolysis: $k = 6.60 \times 10^9$ M$^{-1}$ s$^{-1}$ (Buxton et al. 1986)

Biodegradation:
Biotransformation:

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

Half-Lives in the Environment:

Air: estimated tropospheric chemical lifetimes, $\tau = 5$ h, 3 d and > 150 d for reactions with OH, NO$_3$ and O$_3$, respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)
### TABLE 16.1.8.4.1
Reported vapor pressures of dimethyl sulfoxide at various temperatures and the coefficients for the vapor pressure equations

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

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<td>(C)</td>
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<td>111.95</td>
</tr>
<tr>
<td>(\Delta H_v)</td>
<td>52.89 kJ/mol</td>
</tr>
</tbody>
</table>

**FIGURE 16.1.8.4.1** Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfoxide.

- **Douglas 1948**
- **Jakli & van Hook 1972**

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16.1.8.5 Dimethyl sulfate

Common Name: Dimethyl sulfate
Synonym: sulfuric acid dimethyl ester, DMS
Chemical Name: dimethyl sulfate
CAS Registry No: 77-78-1
Molecular Formula: C₂H₆O₄S, CH₃O-SO₂-OCH₃
Molecular Weight: 126.132
Melting Point (°C): 
-27 (Lide 2003)
Boiling Point (°C): 
188 (decomposes, Lide 2003)
Density (g/cm³ at 20°C): 
1.3322 (Dean 1985)
Molar Volume (cm³/mol): 
95.0 (20°C, Stephenson & Malanowski 1987)
109.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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):
28000 (hydrolyzes, Verschueren 1983; Dean 1985)
28000 (18°C, Budavari 1989)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
< 133 (20°C, Verschueren 1983)
128 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_/kPa) = 7.28235 – 2437.54/(T/K), temp range 340–470 K, (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 33.9406 – 3.853 × 10³/(T/K) – 8.5921·log (T/K) – 1.1705 × 10⁻¹⁰·(T/K) + 8.226 × 10⁻⁷·(T/K)²;
   temp range 241–758 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
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, t½:
   Volatilization:
   Photolysis:
   Oxidation: atmospheric photooxidation t½ = of 36.5–365 h, based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).
   Hydrolysis: first order hydrolysis rate constant k = 1.6 × 10⁻⁴ s⁻¹ at pH 7 and 25°C with t½ = 1.2 h (Mabey & Mill 1978; quoted, Howard et al. 1991).
Biodegradation: aqueous aerobic biodegradation $t_{1/2} \sim 168–672$ h and aqueous anaerobic biodegradation $t_{1/2} \sim 672–2688$ h (Howard et al. 1991).

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

Half-Lives in the Environment:
Air: $t_{1/2} = 36.5–365$ h, based on photooxidation half-life in air from estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime (reaction with liquid water) estimated to be $< 1$ d (Kelly et al. 1994).
Surface water: $t_{1/2} = 1.2–12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).
Groundwater: $t_{1/2} = 1.2–12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).
Sediment:
Soil: $t_{1/2} = 1.2–12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Howard et al. 1991).
Biota:
16.1.8.6 Methanethiol

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

Common Name: Methanethiol  
Synonym: methyl mercaptan  
Chemical Name: methanethiol  
CAS Registry No: 74-93-1  
Molecular Formula: \( \text{CH}_4\text{S}, \text{CH}_3\text{SH} \)  
Molecular Weight: 48.108  
Melting Point (°C):  
\(-123\) (Weast 1982–83; Lide 2003)  
Boiling Point (°C):  
5.9 (Lide 2003)  
Density (g/cm³):  
0.8665 (20°C, Weast 1982–83)  
Dissociation Constant, \( \text{pK}_a \):  

Molar Volume (cm³/mol):  
\( 55.3 \quad (20°C, \text{Stephenson & Malanowski 1987}) \)  
\( 55.2 \quad (\text{calculated-Le Bas method at normal boiling point}) \)  

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
23.8, 24.57 (25, bp, Zwolinski & Wilhoit 1971)  
Enthalpy of Sublimation, \( \Delta H_{\text{subl}} \) (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 (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), \( F \): 1.0  

Water Solubility (g/m³ or mg/L at 25°C):  
39000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny 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):  
101410* (5.977°C, static method-Hg manometer, measured range –51.3 to 5.977°C, Russell et al. 1942)  
log (P/mmHg) = 18.27429 – 1769.05/(T/K) – 3.70248 ± log (T/K); temp range 221.88–279.137 K (static method, Russell, et al. 1942)  
101325* (8.7°C, summary of literature data, temp range –90.7 to 7.8°C, Stull 1947)  
202117* (extrapolated, summary of literature data, temp range –70.3 to 5.956°C, Zwolinski & Wilhoit 1971)  
log (P/mmHg) = 7.03163 – 1015.547/(238.706 + t°C); temp range –70.3 to 24.694°C (Antoine eq., Zwolinski & Wilhoit 1971)  
202346 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)  
log (P/kPa) = 6.18991 – 1030.496/(248.330 + t°C), temp range –51.28 to 5.977°C, (Antoine eq. derived from Russell et al. 1942 data, Boublik et al. 1984)  
log (P/kPa) = 6.19283 – 1031.216/(–32.916 + T/K), temp range 221–283 K, (Antoine eq.-I, Stephenson & Malanowski 1987)  
log (P/kPa) = 6.19219 – 1030.918/(–32.845 + T/K), temp range 222–279 K, (Antoine eq.-II, Stephenson & Malanowski 1987)  
log (P/kPa) = 6.53487 – 1278.361/(5.318 + T/K), temp range 345–424 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):

247  (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)

$\log (1/K_{AW}) = 1347.1/(T/K) – 3.537$; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)

187  (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

300  (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.249 – 1219/(T/K)$, (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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, $t_\frac{1}{2}$:

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:

$k_{OH} = 3.39 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 299.8 K, measured range 300–423 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

$k_{OH}^* = 3.37 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 244–366 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

$k_{OH} = 9.7 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 K (relative rate method, Cox & Sheppard 1980)

$k_{OH} = 2.01 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 293 K (discharge flow-EPR, MacLeod et al. 1983)

$k_{OH} = 2.56 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (discharge flow-RF, Lee & Tang 1983)

$k_{OH}^* = (3.04 – 32.5) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 254–430 K ((flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH}^* = 3.31 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{NO3} = 9.2 \times 10^{-13}$ cm$^3$ ± molecule$^{-1}$ s$^{-1}$, independent of temperature over the range 250–370 K (IUPAC recommended, Atkinson et al. 1989)

$k_{NO3} = 9.3 \times 10^{-13}$ cm$^3$ ± molecule$^{-1}$ s$^{-1}$, independent of temperature over the range 254–367 K (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:
TABLE 16.1.8.6.1
Reported vapor pressures of methanethiol at various temperatures and the coefficients for the vapor pressure equations

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

Russell et al. 1942

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Stull 1947

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Zwolinski & Wilhoit 1971

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FIGURE 16.1.8.6.1 Logarithm of vapor pressure versus reciprocal temperature for methanethiol.
16.1.8.7  Ethanethiol

\[ \text{H}_2\text{S} \]

Common Name: Ethanethiol
Synonym: ethyl mercaptan, thioethyl alcohol, ethylhydrosulfide
Chemical Name: ethanethiol
CAS Registry No: 75-08-1
Molecular Formula: C₂H₆S, C₂H₅SH
Molecular Weight: 62.134
Melting Point (°C):
   -147.88  (Lide 2003)
Boiling Point (°C):
   35.0  (Stull 1947; Dreisbach 1961; Weast 1982–83; Boublík et al. 1984; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
   0.83914, 0.83316 (20°C, 25°C, Dreisbach 1961)
   0.8391  (Weast 1982–83)
   0.8315  (25°C, Dean 1985)
Molar Volume (cm³/mol):
   74.0  (20°C, calculated-density)
   77.4  (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
   27.30, 26.78  (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, \( \Delta H_f \) (kJ/mol):
Entropy of Fusion, \( \Delta S_f \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_f = 56 \) J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   15600  (Hine & Mookerjee 1975)
   12000  (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)
   15000  (Verschueren 1983)
   6800   (Dean 1985)
   6760   (20°C, Budavari 1989)
   14800  (selected, Yaws et al. 1990)
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):
   74630*  (interpolated-regression of tabulated data, temp range –76.7 to 35°C, Stull 1947)
   70110*  (24.933°C, ebulliometric method, measured range 0.405–66.14°C, McCullough et al. 1952)
\[ \log (P/\text{mmHg}) = 6.95206 – \frac{1084.531}{231.385 + t/°C}; \text{temp range 0.405–66.14°C (Antoine eq., ebulliometric method, McCullough et al. 1952)} \]
   70300  (calculated from determined data, Dreisbach 1961)
\[ \log (P/\text{mmHg}) = 6.95206 – \frac{1084.531}{231.385 + t/°C}; \text{temp range –40 to 100°C (Antoine eq. for liquid state, Dreisbach 1961)} \]
\[ \log (P/\text{mmHg}) = 6.95205 – 1084.531/(T/K + 231.385) \]  (Antoine eq., Osborn & Douslin 1966)
\[ 66660*, 70290 (23.613°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971) \]
\[ \log (P/\text{mmHg}) = 6.95026 – 1084.531/(231.385 + t/°C); \text{temp range –49.2 to 55.83°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)} \]
   70320  (calculated-Antoine eq. of Boublík et al. 1973, Przyjazny et al. 1983)
   58660  (20°C, Verschueren 1983)
   70290  (interpolated-Antoine eq., Boublík et al. 1984)
\[ \log (P/kPa) = 6.0768 – 1084.455/(231.374 + t/°C); \text{temp range 0.405–66.115°C (Antoine eq. from reported expctl. data of McCullough et al. 1952, Boublík et al. 1984)} \]
   70300  (calculated-Antoine eq., Dean 1985, 1992)
Nitrogen and Sulfur Compounds

\[ \log (P/\text{mmHg}) = 6.95206 - 1084.531/(231.39 + t/°C); \text{ temp range } -49 \text{ to } 56°C \text{ (Antoine eq., Dean 1985, 1992)} \]

\[ \log (P/\text{kPa}) = 6.07243 - 1081.984/(-42.085 + T/K), \text{ temp range } 273-340 \text{ K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log (P \text{ L/kPa}) = 6.08253 - 1086.982/(-41.517 + T/K), \text{ temp range } 273-313 \text{ K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

\[ \log (P \text{ L/kPa}) = 6.10279 - 1099.374/(-39.807 + T/K), \text{ temp range } 303-448 \text{ K (Antoine eq.-IV, Stephenson & Malanowski 1987)} \]

\[ \log (P \text{ L/kPa}) = 6.42565 - 1328.598/(-6.231 + T/K), \text{ temp range } 365-448 \text{ K (Antoine eq.-V, Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{mmHg}) = 29.2763 - 2.2725 \times 10^3/(T/K) - 7.7769 \cdot \log (T/K) - 3.8954 \times 10^{-11} \cdot (T/K) + 3.517 \times 10^{-6} \cdot (T/K)^2; \text{ temp range } 125-499 \text{ K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
278.1 (exptl., Hine & Mookerjee 1975)
298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
451 (20°C, headspace-GC, Vitenberg et al. 1975)
360.3 (distilled water, headspace-GC/FID, measured range 25-70°C, data in graph, Przyjazny et al. 1983)
\[ \log (1/K_{AW}) = 1486.1/(T/K) - 4.147; \text{ temp range } 25-70°C \text{ (headspace-GC, Przyjazny et al. 1983)} \]
292.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
278, 96.44 (quoted, calculated-molecular structure, Russell et al. 1992)
292.5 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
\[ \log K_{AW} = 4.147 - 1486/(T/K) \text{ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)} \]

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

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, \( t_{1/2} \):

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 and the Arrhenius expression see reference:
\[ k_{OH} = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for gas-phase reaction with O}^+(\text{P}) \text{ atom at } 298 \text{ K, measured range } 257-495 \text{ K} \text{ (Slagle et al. 1978)} \]
\[ k_{OH} = 3.67 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K} \text{ (discharge flow-RF, Lee & Tang 1983)} \]
\[ k_{OH} = 2.70 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 293 \text{ K} \text{ (discharge flow-EPR, Mac Leod et al. 1984)} \]
\[ k_{OH}^* = 4.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 252-425 \text{ K (flash photolysis-resonance fluorescence, Wine et al. 1984)} \]
\[ k_{OH}^* = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1985)} \]
\[ k_{OH} = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K (relative rate method, Barnes et al. 1986)} \]
\[ k_{OH}^* = 4.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)} \]
\[ k_{NO3} = (1.21 \pm 0.28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{K (relative rate method, Mac Leod et al. 1986; quoted, Atkinson 1991)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
TABLE 16.1.8.7.1
Reported vapor pressures of ethanethiol at various temperatures and the coefficients for the vapor pressure equations

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

(1) \hspace{1cm} \text{ln } P = A - B/(T/K) \hspace{1.2cm} (1a)

(2) \hspace{1cm} \text{ln } P = A - B/(C + t/°C) \hspace{1.2cm} (2a)

(3)

(4)

Summary of literature data

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FIGURE 16.1.8.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanethiol.
16.1.8.8 1-Propanethiol

Common Name: 1-Propanethiol
Synonym: n-propyl mercaptan, 1-mercaptopropane
Chemical Name: 1-propanethiol
CAS Registry No: 107-03-9
Molecular Formula: C₃H₈S, CH₃CH₂CH₂SH
Molecular Weight: 76.171
Melting Point (°C):
   –113.13  (Lide 2003)
Boiling Point (°C):
   67.8  (Lide 2003)
Density (g/cm³):
   0.8411  (20°C, Weast 1982–83)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ∆HV (kJ/mol):
   31.88, 29.53 (25°C, bp, Zwolinski & Wilhoit 1971)
Enthalpy of Sublimation, ∆Hsubl (kJ/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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   3800  (estimated-activity coefficient by headspace-GC/FID, Przyjazny 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):
   13332*  (15.3°C, summary of literature data, temp range –56.0 to 67.4°C, Stull 1947)
   19920*  (24.275°C, ebulliometry, measured range 24.3–102.088°C, Pennington et al. 1956)
   log (P/mmHg) = 6.92846 – 1183.307/(T/K + 224.624); temp range 24.3–102.088°C (Antoine eq., ebulliometry, Pennington et al. 1956; Osborn & Douslin 1966)
   20558*  (interpolated-Antoine eq., temp range –25 to 90.73°C, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.92846 – 1183.307/(224.624 + t/°C); temp range –25 to 90.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
   20569  (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
   log (P/kPa) = 6.05331 – 1183.265/(224.618 + t/°C), temp range 24.27–102.088°C (Antoine eq. derived from Pennington et al. 1956 data, Boublik et al. 1984)
   log (P/kPa) = 6.05019 – 1181.703/(–48.687 + T/K), temp range 296–376 K, (Antoine eq., Stephenson & Malanowski 1987)
   log (P/mmHg) = 6.92846 – 1183.307/(224.62 + t/°C), temp range –25 to 91°C (Antoine eq., Dean 1992)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
   414  (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
   log (1/Kₐᵥ) = 1552.2/(T/K) – 4.428; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
   331  (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
   log Kₐᵥ = 4.428 – 1552/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log Kₒₐᵥ:
   1.81  (shake flask, Log P Database, Hansch & Leo 1987)
   1.81  (recommended, Sangster 1993)
   1.81  (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, $t_{1/2}$;

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 $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH}^* = (4.18–4.56) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 257–419 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

### TABLE 16.1.8.8.1
Reported vapor pressures of 1-propanethiol at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
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**Stull 1947**

**Pennington et al. 1956**

**Zwolinski & Wilhoit 1971**

Summary of literature data

Ebulliometry

Selected values
TABLE 16.1.8.8.1 (Continued)

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<th>P/Pa</th>
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<th>P/Pa</th>
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<td>eq. 2</td>
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<td>data also fitted to Cox eq.</td>
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\[ \Delta H_v/(kJ \text{ mol}^{-1}) = \]
- at 25°C: 31.88
- at bp: 29.53

FIGURE 16.1.8.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1-propanethiol.
16.1.8.9  1-Butanethiol (Butyl mercaptan)

Common Name: 1-Butanethiol
Synonym: butyl mercaptan, n-butyl mercaptan
Chemical Name: 1-butanethiol
CAS Registry No: 109-79-5
Molecular Formula: C₄H₁₀S, CH₃(CH₂)₃SH
Molecular Weight: 90.187
Melting Point (°C):
-115.7 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
98.5 (Lide 2003)
Density (g/cm³ at 25°C):
0.8337 (20°C, Weast 1982–83)
0.84159, 0.83674 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
107.8 (calculated-density, Stephenson & Malanowski 1987)
121.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ;
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
36.53, 32.225 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fu} \) (kJ/mol):
10.46 (Riddick et al. 1986)
Entropy of Fusion, \( \Delta S_{fu} \) (J/mol K);
Fugacity Ratio at 25°C (assuming \( \Delta S_{fu} = 56 \) J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
597 (Riddick et al. 1986)
600 (selected, Yaws et al. 1990)
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):
19920* (51.409°C, ebulliometry, measured range 51.4–135.7°C, Scott et al. 1957)
log (P/mmHg) = 6.92754 – 1281.018/(T/K + 218.100) (Antoine eq., Osborn & Douslin 1966)
5330*, 6070 (22.4°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.92754 – 1281.018/(218.10 + t°C); temp range –2.0 to 123.37°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
log (P/kPa) = 6.05296 – 1281.344/(218.139 + t°C); temp range 51.409–135.7°C (Antoine eq. derived from Scott et al. 1957 data, Boublik et al. 1984)
6070 (Riddick et al. 1986)
log (P/kPa) = 6.05244 – 1281.018/(218.10 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 6.05011 – 1279.95/(-55.132 + T/K), temp range 323–409 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 6.92754 – 1281.018/(218.10 + t°C), temp range –2 to 123°C (Antoine eq., Dean 1992)
log (P/mmHg) = 36.2672 – 3.0452 × 10³/(T/K) –9.9743·log (T/K) – 9.1432 × 10⁻¹¹·(T/K)², temp range 157–569 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
460.7 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
log (1/K₂ₐ) = 1655.9/(T/K) – 4.823; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
911.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
363 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K₂ₐ = 4.823 – 1656/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.28 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.28 (recommended, Sangster 1989)
- 2.28 (recommended, Hansch et al. 1995)

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, $t_\text{1/2}$:
- 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$_3$ as indicated; *data at other temperatures see reference:
  - $k_{OH} = 4.21 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{OH} = 4.55 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wine et al. 1984)
  - $k_{OH} = 5.82 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (relative rate method, Barnes et al. 1986)
  - $k_{OH} = 5.11 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

### TABLE 16.1.8.9.1
Reported vapor pressures of 1-butanol at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>$\Delta H^\circ/(kJ mol^{-1}) = \ $</th>
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<td>51.409</td>
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<td>57.130</td>
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<td>62.897</td>
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<td>68.710</td>
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<td>74.567</td>
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<table>
<thead>
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</table>

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FIGURE 16.1.8.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butanol.

1-Butanethiol: vapor pressure vs. 1/T

b.p. = 98.5 °C

Scott et al. 1957
Zwolinski & Wilhoit 1971
16.1.8.10 Benzenethiol

Common Name: Benzenethiol
Synonym: thiophenol, phenyl mercaptan, mercaptobenzene
Chemical Name: benzenethiol
CAS Registry No: 108-98-5
Molecular Formula: C₆H₆S, C₆H₅SH
Molecular Weight: 110.177
Melting Point (°C):
  -14.93 (Lide 2003)
Boiling Point (°C):
  169.1 (Lide 2003)
Density (g/cm³):
  1.0766 (20°C, Weast 1982–83)
Dissociation Constant, pKₐ:
  6.615 (Riddick et al. 1986)
Molar Volume (cm³/mol):
  102.7 (calculated-density, Stephenson & Malanowski 1987)
  106.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
  45.35, 36.97 (25°C, bp, Riddick et al 1986)
Enthalpy of Sublimation, ΔHₛᵤₙ (kJ/mol):
  11.45 (calorimetry at triple pt 258.27 K, Scott et al. 1956)
  11.447 (Riddick et al. 1986)
Entropy of Fusion, ΔSₕᵤₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕᵤₛ = 56 J/mol K), 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):

133* (18.6°C, summary of literature data, temp range 18.6–168°C, Stull 1947)
1333* (51.5°C, ebulliometry, measured range 51.5–167.0°C, Vonderres et al. 1955)
\[ \log (P/\text{mmHg}) = 6.99019 - 1529.454/(230.048 + t/°C) \]; temp range 114.5–212°C (comparative ebulliometry, data fitted to Antoine eq., Scott et al. 1956)
\[ \log (P/\text{mmHg}) = A \pm [1 - 442.298/(T/K)], \text{ where } A = 0.87370 - 6.4975 \times 10^{-4} \pm (T/K) + 5.2309 \times 10^{-7} \pm (T/K)^2; \text{ measured range 114.5–212°C (data fitted to Cox eq., comparative ebulliometry, Scott et al. 1956) } \]
1333* (52.28°C, derived from compiled data, temp range 52.3–198°C, Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 6.99019 - 1529.454/(230.048 + t/°C) \]; temp range 52.3–198°C (Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/kPa) = 6.11539 - 1529.668/(203.074 + t/°C), \text{ temp range 114.5–212.16°C (Antoine eq. derived from Scott et al. 1956 data, Boublik et al. 1984) } \]
397 (selected, Riddick et al. 1986)
\[ \log (P/kPa) = 6.11509 - 1529.46/(t/°C + 258.21); \text{ temp range not specified (Antoine eq., Riddick et al. 1986) } \]
\[ \log (P/\text{kPa}) = 6.11531 - 1530.286/(-69.948 + T/K); \text{ temp range 385–486 K (Antoine eq., Stephenson & Malanowski 1987) } \]
\[ \log (P/\text{mmHg}) = -5.4919 \times 10^3/(T/K) + 8.1770 \log (T/K) - 1.9494 \times 10^{-2}(T/K) + 9.2817 \times 10^{-6}(T/K)^2; \text{ temp range 258–69 K (vapor pressure eq., Yaws et al. 1994) } \]
Henry’s Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
- 2.52 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.52 (recommended, Sangster 1989)
- 2.52 (recommended, Hansch et al. 1995)

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, $t_\text{1/2}$:

Half-Lives in the Environment:

### TABLE 16.1.8.10.1
Reported vapor pressures of benzenethiol at various temperatures and the coefficients for the vapor pressure equations

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<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>(1) log P = A – B/(T/K)</th>
<th>(1a) ln P = A – B/(T/K)</th>
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<th>(3) log P = A – B/(C + T/K)</th>
<th>(4) log P = A – B/(T/K) – C·log (T/K)</th>
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<td>at normal bp</td>
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</table>

**FIGURE 16.1.8.10.1** Logarithm of vapor pressure versus reciprocal temperature for benzenethiol.
16.1.8.11 Thiophene

Common Name: Thiophene
Synonym: thiofuran
Chemical Name: thiophene, thiofuran
CAS Registry No: 110-02-1
Molecular Formula: C₄H₄S
Molecular Weight: 84.140
Melting Point (°C):
-38.21 (Lide 2003)
Boiling Point (°C):
84.0 (Lide 2003)
Density (g/cm³ at 20°C):
1.06485, 1.05887 (20°C, 25°C, Dreisbach 1955)
1.0649 (Weast 1982–83)
1.06482, 1.05884 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
79.0 (20°C, calculated from density)
88.10 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Vaporization, ΔHV (kJ/mol):
34.6, 31.472 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
5.088 (Riddick et al. 1986)
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):
3015 (shake flask-GC, Price 1976)
3900 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)
3600 (18°C, Verschueren 1983)
3020 (selected, Yaws et al. 1990)
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):
9670* (interpolated-regression of tabulated data, temp range -40.7 to 81.4°C, Stull 1947)
7998 (20.1°C, Stull 1947)
10622* (ebulliometry and manometry, measured range 0–84.155°C, Waddington et al. 1949)
10620 (calculated from determined data, Dreisbach 1955)
log (P/mmHg) = 6.95926 – 1246.038/(221.354 + t°C), temp range 5–155°C (Antoine eq. for liquid state, Dreisbach 1955)
482307* (148.89°C, static-Bourdon gauge, measured range 148.89–304.44°C, Kobe et al. 1956)
44930* (60.3 °C, isoteniscope/manometry, measured range 60.3–100.3 °C, Eon et al. 1971)
10670, 10660* (25.09°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.95926 – 1246.01/(221.35 + t°C); temp range –12.3 to 108.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 8748.3/(T/K)] + 8.273276; temp range –40.7 to 84.4°C (Antoine eq., Weast 1972–73)
2450 (calculated-Cox eq., Chao et al. 1983)
log (P/atm) = [1 – 394.395/(T/K)] × 10^4[0.901276 – 10.3229 × 10^4 ± (T/K) + 21.9193 × 10^7 ± (T/K)^2]; temp range: 278.35–443.60 K (Cox eq., Chao et al. 1983)
log (P/kPa) = 6.1336 – 1260.606/(222.787 + t/°C), temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.08467 – 1246.02/(221.35 + t/°C), temp range 39.9–119.79°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.0723 – 1138.803/(220.477 + t/°C), temp range not specified (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.95926 – 1246.02/(221.35 + t/°C), temp range –12 to 108°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 36.6016 – 2.9794 × 10³/(T/K) – 10.104·log (T/K) + 1.1445 × 10⁻⁶·(T/K)²; temp range 235–579 K (vapor pressure eq., Yaws et al. 1994)

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

log (1/KAW) = 1563.6/(T/K) – 4.199; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

log (1/KAW) = 1580.0/(T/K) – 4.277; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

log (1/KAW) = 1661.9/(T/K) – 4.542; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)

224, 236, 230 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)

log (1/KAW) = 1653.6/(T/K) – 4.199; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

log (1/KAW) = 1580.0/(T/K) – 4.277; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

log (1/KAW) = 1661.9/(T/K) – 4.542; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)

223.3 (calculated-PIC with selected values)

296 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

182 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log KAw = 4.542 – 1662/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kow:

1.81 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.79 (calculated-f const., Rekker 1977)

1.74 (HPLC-RV correlation, Garst 1984)

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

1.81 (recommended, Sangster 1989, 1993)

1.82 (shake flask-UV, Yamagami & Takao 1992)

1.81 (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, or 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 the Arrhenius expression see reference:
Nitrogen and Sulfur Compounds

\[ k_{\text{OH}} = (9.58 \pm 0.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with calculated atmospheric lifetime \( \tau \approx 28 \text{ h} \); and \( k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 ± 2 K and \( k_{\text{O}_3(3P)} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for reaction with O(3P) atom at room temp. (relative rate method, Atkinson et al. 1983)

\[ k_{\text{OH}} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a loss rate of < 0.004 d\(^{-1}\), \( k_{\text{OH}} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a loss rate of 0.8 d\(^{-1}\); \( k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a loss rate of 0.7 d\(^{-1}\) at room temp. (review, Atkinson & Carter 1984)

\[ k_{\text{OH}} = (9.37, 9.57) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, measured range 255–425 K (flash photolysis-resonance fluorescence, Wine & Thompson 1984)

\[ k_{\text{OH}} = 9.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (recommended, Atkinson 1985)

\[ k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a loss rate of < 0.004 d\(^{-1}\), \( k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a loss rate of 0.4 d\(^{-1}\), and \( k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a loss rate of 0.7 d\(^{-1}\) at room temp. (review, Atkinson 1985)

\[ k_{\text{NO}_3} = (3.2 \pm 0.7) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a calculated lifetime of 36 h and a loss rate of 0.7 d\(^{-1}\) assuming \( 2.4 \times 10^8 \text{ NO}_3 \) radicals/cm\(^3\) in nighttime air at 295 ± 1 K in the atmosphere (relative rate technique, Atkinson et al. 1985)

\[ k_{\text{OH}} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a calculated tropospheric lifetime \( \tau > 270 \text{ d} \), \( k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated lifetime of 29 h during daytime hours, and \( k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated lifetime of 36 h at room temp. (review, Atkinson 1985)

\[ k_{\text{OH}}^* = 9.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (recommended, Atkinson 1989)

\[ k_{\text{NO}_3} = 3.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] independent of temperature over the range 272–296 K (recommended, Atkinson 1991)

\[ k_{\text{OH}}(\text{calc}) = 14.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at room temp. (molecular orbital calculations, Klamt 1993)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Air: atmospheric lifetime of ~28 h due to reactions with OH radical (Atkinson et al. 1983); calculated gas-phase lifetime of 29 h for the reaction with OH radical during daytime hours, calculated lifetime of 36 h for reaction with NO\(_3\) radical and a calculated lifetime > 270 d for reaction with O\(_3\) at room temp. (Atkinson et al. 1985)

### TABLE 16.1.8.11.1
Reported vapor pressures of thioephene at various temperatures and the coefficients for the vapor pressure equations

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<td>selected values</td>
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<td>( T/°C )</td>
<td>( P/Pa )</td>
<td>( T/°C )</td>
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(Continued)
TABLE 16.1.8.11.1 (Continued)

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<tr>
<td>ΔHv/(kJ mol⁻¹) = 34.77</td>
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<tr>
<td>ΔHv/(kJ mol⁻¹) =</td>
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<td>at 45.36°C</td>
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<td>at bp</td>
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<td>32.67</td>
<td>304.44</td>
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FIGURE 16.1.8.11.1 Logarithm of vapor pressure versus reciprocal temperature for thiophene.
16.1.8.12 Benzo[b]thiophene

![Chemical Structure]

**Common Name:** Benzo[b]thiophene  
**Synonym:** thianaphthene, thionaphthene, 1-benzothiophene  
**Chemical Name:**  
**CAS Registry No:** 95-15-8  
**Molecular Formula:** C₈H₆S  
**Molecular Weight:** 134.199  
**Melting Point (°C):**  
32  
(Lide 2003)  
**Boiling Point (°C):**  
221  
(Lide 2003)  
**Density (g/cm³ at 20°C):**  
1.1500  
(Verschueren 1983)  
**Molar Volume (cm³/mol):**  
139.7  
(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:** 0.854 (mp at 32°C)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
130.0  
(20°C, shake flask, Smith et al. 1978)  
130.2  
(Mill et al. 1981)  
216*  
(59.05°C, equilibrium cell-GC, measured range 332.2–490.5 K, Leet et al. 1987)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
26.7  
(20°C, estimated from naphthalene, Smith et al. 1978)  
14.80  
(calculated-bp, Mackay et al. 1982)  
log (P/mmHg) = –9.5352 – 2.6947 × 10³/(T/K) + 8.8858·log (T/K) – 1.5478 · 10⁻²·(T/K)²; temp range 305–754 K (vapor pressure eq., Yaws 1994)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
28.0  
(calculated-P/C, Smith & Bomberger 1980)  
24.1  
(calculated-P/C, this work)  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
3.09  
(shake flask-UV, pH 7.4, Rogers & Cammarata 1969)  
3.05  
(HPLC-RT correlation, De Voogt et al. 1988)  
3.12  
(recommended, Sangster 1989, 1993)  
3.26  
(shake flask-HPLC, De Voogt et al. 1990)  
3.18  
(HPLC-RT correlation, Ritter et al. 1994)  
3.17  
(shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)  
**Octanol/Air Partition Coefficient, log K_{oa}:**  
**Bioconcentration Factor, log BCF:**  
2.08  
(mixed microbial populations, Steen & Karickhoff 1981)  
**Sorption Partition Coefficient, log K_{oc}:**  
1.77  
(Coyote Creek sediment, Smith et al. 1978)  
2.30  
/lab. mixture of microorganisms, Smith et al. 1978)  
3.49, 3.0  
(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ hours in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7}$ s$^{-1}$ exposed to 12 h sunlight per day in late May with estimated $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Oxidation:
- Laboratory investigated $k = 83$ M$^{-1}$ s$^{-1}$ for the reaction with RO$_2$ radical and estimated $t_{1/2} = 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
- $k = 5.7 \times 10^{-6}$ s$^{-1}$ with $t_{1/2} = 34$ h under natural sunlight conditions, $k = 83$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 96$ d for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{1/2} > 20$ h in river, $t_{1/2} < 20$ h in eutrophic pond, $t_{1/2} = 20$ h in eutrophic lake and very long half-life in oligotrophic lake, based on the biodegradation rate in the presence of alternative carbon sources will be one-half the biodegradation rate of quinoline when quinoline is the only carbon source by the one compartment model (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: estimated volatilization $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978);

photolysis rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7}$ s$^{-1}$ exposed to 12 h sunlight per day in late May with estimated photolysis $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).
16.1.8.13 Dibenzothiophene

![Chemical structure of Dibenzothiophene](image)

Common Name: Dibenzothiophene
Synonym: dibenzothiophene
Chemical Name: dibenzothiophene
CAS Registry No: 132-65-0
Molecular Formula: C_{12}H_{8}S
Molecular Weight: 184.257
Melting Point (°C):
98.2 (Lide 2003)
Boiling Point (°C):
332.5 (Lide 2003)
Density (g/cm³ at 20°C):
191.3 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.191 (mp at 98.2°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1.11 ± 0.09 (28°C, measured, Smith et al. 1978)
1.470 (24°C, shake flask-LSC, Means et al. 1980)
1.106 (Mill et al. 1981)
1.500 (Steen & Karickhoff 1981)
1.032 (literature average, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.267 (20°C, estimated, Aubry et al. 1975)

log (P/mmHg) = 22.90 – 10910/(T/K), temp range 60–00°C (solid, gas saturation, Edward & Prausnitz 1981)
log (P/mmHg) = 21.10 – 8353/(T/K), temp range 100–130°C (liquid, gas saturation, Edward & Prausnitz 1981)
0.263, 0.0083 (20°C, quoted, calculated-bp, Mackay et al. 1982)
0.893 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1982)
0.586 (extrapolated-Cox eq., Chao et al. 1983)

log (P/atm) = [1– 605.160/(T/K)] × 10^{0.865373 – 5.51221 × 10^{-2} ± (T/K) + 6.05701 × 10^{-7} ±(T/K)^{2}}; temp range: 424.81–607.53 K (Cox eq., Chao et al. 1983)
log (P/kPa) = 7.18577 – 3140.15/(T/K), temp range 385–574 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
44.3 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log K_{ow}:
4.38 (shake flask-LSC, Means et al. 1980)
4.33 (HPLC-RT correlation, De Voogt et al. 1988)
4.38 (recommended, Sangster 1989, 1993)
4.49 (shake flask-HPLC, De Voogt et al. 1990)
4.38 (recommended, Hansch et al. 1995)
4.41 ± 0.19, 4.43 ± 0.61 (HPLC-k’ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
4.36 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)

Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
3.20 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log $K_{oc}$:
3.14 (Coyote Creek sediment, Smith et al. 1978)
4.05 (soil, Hassett et al. 1980)
4.05 (average of 3 sediment/soil samples, equilibrium sorption isotherm, Means et al. 1980)
4.00 (soil, calculated-MCI $\chi$, Sabljic 1987)
4.00 (soil, calculated-MCI $\chi$, Sabljic 1987)
4.17 (soil, calculated-$K_{ow}$, model of Karickhoff et al. 1979, Sabljic 1987)
3.75 (soil, calculated-$K_{ow}$, model of Kenaga & Goring 1980, Sabljic 1987)
2.92 (soil, calculated-$K_{ow}$, model of Briggs 1981, Sabljic 1987)
4.00 (soil, calculated-$K_{ow}$, model of Means et al. 1982, Sabljic 1987)
3.60 (soil, calculated-$K_{ow}$, model of Chiou et al. 1983, Sabljic 1987)
4.59 (humic acid, HPLC $k'$ correlation, Nielsen et al. 1997)
3.87 (soil: organic carbon $OC \geq 0.1\%$, average, Delle Site 2001)
4.02, 4.04 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
4.07 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

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

Volatilization: estimated $t_\frac{1}{2} = 140$ h in river, $t_\frac{1}{2} = 720$ h in eutrophic pond, $t_\frac{1}{2} = 580$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: solar photolysis $k = 1.5 \times 10^{-8}$ s$^{-1}$ over 24-h day; rate constant of transformation and transport of $(2.04 \pm 0.08) \times 10^{-6}$ s$^{-1}$ exposed to 12 h sunlight per day in early March with estimated $t_\frac{1}{2} = 380$ h in river, $t_\frac{1}{2} = 950$ h in eutrophic pond and eutrophic lake and $t_\frac{1}{2} = 190$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978); $t_\frac{1}{2} = 4–8$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation: laboratory investigated $k < 7.5$ M$^{-1}$ s$^{-1}$ for the reaction with RO$_2$ radical and estimated $t_\frac{1}{2} > 10^5$ h in river, eutrophic pond, eutrophic lake, and oligotrophic lake by the one compartment model (Smith et al. 1978). $k = 1.5 \times 10^{-6}$ s$^{-1}$ with $t_\frac{1}{2} = 128$ h under natural sunlight conditions, $k < 7.5$ M$^{-1}$ s$^{-1}$ with $t_\frac{1}{2} > 3.5$ yr for free-radical oxidation in air-saturated water (NRCC 1983).

Hydrolysis:
Biodegradation: $k = 5.3 \times 10^{-7}$ mL cell$^{-1}$ h$^{-1}$ and the estimated $t_\frac{1}{2} = 13$ h in river, eutrophic pond, and eutrophic lake and $t_\frac{1}{2} > 10^4$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

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

Half-Lives in the Environment:
Surface water: $t_\frac{1}{2} = 0.5$ h from river water, $t_\frac{1}{2} = 13$ h from pond water, $t_\frac{1}{2} = 13$ h from eutrophic lake and $t_\frac{1}{2} = 140$ h from oligotrophic lake predicted by one-compartment model for all processes; estimated volatilization $t_\frac{1}{2} = 140$ h in river, $t_\frac{1}{2} = 720$ h in eutrophic pond, $t_\frac{1}{2} = 580$ h in eutrophic lake and oligotrophic lake; photolysis rate constant of transformation and transport $k = (2.04 \pm 0.08) \times 10^{-6}$ s$^{-1}$ exposed to 12 h sunlight per day in early March with estimated photolysis $t_\frac{1}{2} = 380$ h in river, $950$ h in eutrophic pond and eutrophic lake and $t_\frac{1}{2} = 190$ h in oligotrophic lake; biodegradation $t_\frac{1}{2} = 13$ h in river, eutrophic pond water and $t_\frac{1}{2} = 140$ h in oligotrophic lake (Smith et al. 1978); $t_\frac{1}{2} = 4–8$ h for disappearance via direct photolysis in aqueous media (Harris 1982).
16.1.8.14 Thiourea

H₂N-S-NH₂

Common Name: Thiourea
Synonym: thiocarbamide
Chemical Name: thiourea
CAS Registry No: 62-56-6
Molecular Formula: CH₄N₂S, H₂NCSNH₂
Molecular Weight: 76.121
Melting Point (°C):
178 (Lide 2003)
Boiling Point (°C):
decomposes (Verschueren 1983)
Density (g/cm³ at 20°C):
1.045 (Weast 1982–83; Verschueren 1983, Dean 1992)
Dissociation Constant, pK:
2.03 (pK₁, Dean 1985)
Molar Volume (cm³/mol):
76.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
14.42 (Donnelly et al. 1990)
12.55 (Kim et al. 1994)
15.64, 14.92, 15.17 (differential scanning calorimetry in three types of crucibles, Gatta et al. 2000)
Entropy of Fusion, ∆S_fus (J/mol K):
35.2, 33.7, 34.1 (Gatta et al. 2000)
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F: 0.0315 (mp at 178°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
910000 (20–25°C, shake flask-gravimetric, Dehn 1917)
918000 (13°C, Verschueren 1983)
89800 (Windholz 1983)
110000 (Budavari 1989)
90000 (Dean 1985)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_ow:
-1.02 (Leo et al. 1971)
-0.95 (shake flask, Cornford 1982)
-2.38, -0.95 (calculated, Verschueren 1983)
-1.08, -1.03 (pH 6.5, pH 12, shake flask-HPLC, Govers et al. 1986)
-1.14, -1.02 (shake flask, Log P Database, Hansch & Loe 1987)
-0.99 (recommended, Sangster 1993)
-1.02 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_oa:

Bioconcentration Factor, log BCF:
1.73 (alga chlorella fusca, wet wt. basis, Geyer et al. 1984)
-0.699 (alga chlorella fusca, calculated-K_ow, Geyer et al. 1984)
Sorption Partition Coefficient, log $K_{OC}$:

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

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 1.6–16$ h in air, based on rate constant for the vapor-phase reaction with OH radical and photooxidation $t_{1/2} = 2048–81927$ h in water, based on estimated rate data for reaction with OH radical in aqueous solution (Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 24–168$ h, based on aqueous aerobic screening test data and aqueous anaerobic biodegradation $t_{1/2} = 96–672$ h, based on aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 1.6–16$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24–168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24–168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:
16.1.8.15 Thioacetamide

\[
\begin{align*}
\text{S} & \quad \text{NH}_2
\end{align*}
\]

Common Name: Thioacetamide
Synonym: ethanethioamide, acetothioamide
Chemical Name: thioacetamide
CAS Registry No: 62-55-5
Molecular Formula: C₂H₅NS, CH₃CSNH₂
Molecular Weight: 75.133
Melting Point (°C): 115.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   84.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔH_m (kJ/mol):
Entropy of Fusion, ΔS_m (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_m = 56 J/mol K), F: 0.129 (mp at 115.5°C)

Water Solubility (g/m³ or mg/L at 25°C):
   163000 (Dean 1985)
   163000 (Budavari 1989)
Vapor Pressure (Pa at 25°C):
Henley’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₜₕw:
   -0.46, 0 36 (Verschueren 1983)
   -0.26 (shake flask, Log P Database, Hansch & Leo 1987)
   -0.26 (recommended, Sangster 1993)
   -0.26 (recommended, Hansch & Leo 1995)
Octanol/Air Partition Coefficient, log Kₜₕₐ:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₜₕₙ:

Environmental Fate Rate Constants, k, or Half-Lives, tₕ:
Volatilization:
   Photolysis:
   Oxidation: atmospheric tₕ = 3.2–31.7 h, based on estimated rate data for OH radical in air (Howard et al. 1991).
   Hydrolysis: first-order rate constant k = 8.6 × 10⁻¹ h⁻¹ at pH 7 and 25°C (Ellington et al. 1987), corresponding to a tₕ = 8064 h (Howard et al. 1991);
   acid rate constant k = 6.0 × 10⁻² M⁻¹ h⁻¹, corresponding to a tₕ = 333 d and base rate constant k = 1.4 M⁻¹ h⁻¹, corresponding to a tₕ = 289 d (Howard et al. 1991).
   Biodegradation: aerobic biodegradation tₕ = 24–168 h, based on aqueous aerobic screening test data and anaerobic biodegradation tₕ = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
   Biotransformation:
   Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
Half-Lives in the Environment:

Air: $t_{1/2} = 3.2–31.7$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24–268$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24–168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
### TABLE 16.2.1
Summary of physical properties of nitrogen and sulfur containing compounds

<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>MW/ρ at 20°C</th>
<th>Le Bas</th>
<th>pK_a or pK_b</th>
<th>Molar volume, V_m cm^3/mol</th>
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<td><strong>Nitriles:</strong></td>
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<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
<td>CH₃CN</td>
<td>41.052</td>
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<td>1</td>
<td>52.25</td>
<td>56.3</td>
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<td>Propionitrile</td>
<td>107-12-0</td>
<td>C₃H₅CN</td>
<td>55.079</td>
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<td>97.14</td>
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<td>78.5</td>
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<td>Butyronitrile</td>
<td>109-74-0</td>
<td>C₄H₇CN</td>
<td>69.106</td>
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<td>1</td>
<td>87.35</td>
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<td>Acrylonitrile (2-Propenitrile)</td>
<td>107-13-1</td>
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<td>53.063</td>
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<td>Adiponitrile</td>
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<td>CN(CH₂)₄CN</td>
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<td><strong>Aliphatic amines:</strong></td>
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<td>Methyamine</td>
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<td>(CH₃)₂NH</td>
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<td>(C₂H₅)₂NH</td>
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<td>Triethylamine</td>
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<td>(C₂H₅)₃N</td>
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(Continued)
### TABLE 16.2.1 (Continued)

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<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>
<th>pK_a or pK_b</th>
<th>MW/ρ at 20°C</th>
<th>Le Bas</th>
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*Continued*
TABLE 16.2.1 (Continued)

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<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>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
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<tr>
<td>2,3-Dimethylpyridine</td>
<td>583-61-9</td>
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**Quinolines:**

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<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Molar volume, V_m cm³/mol</th>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
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<tr>
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<td>61</td>
<td>264.5</td>
<td>0.443</td>
<td></td>
<td>189.1</td>
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<tr>
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<td>85-02-9</td>
<td>C₈H₁₀N</td>
<td>179.217</td>
<td>94</td>
<td>352</td>
<td>0.210</td>
<td></td>
<td>196.3</td>
<td></td>
</tr>
<tr>
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<td>230-27-3</td>
<td>C₉H₁₁N</td>
<td>179.217</td>
<td>52</td>
<td>339</td>
<td>0.543</td>
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**9H-Carbazole**

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<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Molar volume, V_m cm³/mol</th>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
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<tr>
<td>2,7-Dimethylquinoline</td>
<td>93-37-8</td>
<td>C₈H₁₀N</td>
<td>157.212</td>
<td>61</td>
<td>264.5</td>
<td>0.443</td>
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<td>189.1</td>
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<tr>
<td>Benzo[f]quinoline</td>
<td>85-02-9</td>
<td>C₈H₁₀N</td>
<td>179.217</td>
<td>94</td>
<td>352</td>
<td>0.210</td>
<td></td>
<td>196.3</td>
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<tr>
<td>Benzo[h]quinoline</td>
<td>230-27-3</td>
<td>C₉H₁₁N</td>
<td>179.217</td>
<td>52</td>
<td>339</td>
<td>0.543</td>
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**7H-Dibenzo[c,g]carbazole**

<table>
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<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>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acridine</td>
<td>260-94-6</td>
<td>C₁₃H₉N</td>
<td>179.217</td>
<td>110</td>
<td>344.86</td>
<td>0.147</td>
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<td>5.60</td>
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<tr>
<td>Benzo[a]acridine</td>
<td>225-11-6</td>
<td>C₁₃H₉N</td>
<td>229.276</td>
<td>132</td>
<td>339</td>
<td>0.543</td>
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<td>196.3</td>
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</tr>
<tr>
<td>Benzo[c]acridine</td>
<td>225-51-4</td>
<td>C₁₃H₉N</td>
<td>229.276</td>
<td>132</td>
<td>339</td>
<td>0.543</td>
<td></td>
<td>196.3</td>
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<tr>
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**Sulfur compounds:**

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<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Molar volume, V_m cm³/mol</th>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon disulfide</td>
<td>75-15-0</td>
<td>CS₂</td>
<td>76.141</td>
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<td></td>
<td>60.28</td>
<td>66.0</td>
</tr>
<tr>
<td>Dimethyl sulfate</td>
<td>77-78-1</td>
<td>(CH₃O)₂SO</td>
<td>126.132</td>
<td>-27</td>
<td>188 dec</td>
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<td>109.7</td>
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<tr>
<td>Diethyl sulfate</td>
<td>64-67-5</td>
<td>(C₂H₅O)₂SO</td>
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<td>208</td>
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<td>138.4</td>
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<tr>
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<td>60.28</td>
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<td>(CH₃)₂SO</td>
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**Thiols:**

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<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>
<th>MW/ρ Le Bas</th>
<th>pK_a or pK_b</th>
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<tr>
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<td>Ethanethiol</td>
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<td>107-03-9</td>
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</tr>
<tr>
<td>1-Butanethiol (Butyl mercaptan)</td>
<td>109-79-5</td>
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<td>90.187</td>
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<td>98.5</td>
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<td>121.8</td>
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<td>Compound</td>
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<td>Molecular Formula</td>
<td>T (°C)</td>
<td>S (mJ/mol K)</td>
<td>V (mL/mol)</td>
<td>Density (g/mL)</td>
<td>Boiling Point (°C)</td>
<td>Melting Point (°C)</td>
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<td>0.129</td>
<td>84.2</td>
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* Assuming ΔSₘₙₐₜ = 56 J/mol K
### TABLE 16.2.2
Summary of selected physical-chemical properties of nitrogen and sulfur containing compounds at 25°C.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Solubility</th>
<th>log $K_{ow}$</th>
<th>Henry's law constant</th>
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<td>$P_5$/Pa</td>
<td>$P_1$/Pa</td>
<td>$S_5/(g/m^3)$</td>
<td>$C_5/(mol/m^3)$</td>
<td>$C_1/(mol/m^3)$</td>
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Nitrogen and Sulfur Compounds

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16.3 REFERENCES


Nitrogen and Sulfur Compounds


GEMS (1986) Graphical Exposure Modeling System. FAP. Fate of Atmospheric Pollutants.


Harris, G.W., Klein, T.E., Pitts, J.N., Jr. (1981) Rate constants for the reaction of OH radicals with CH$_3$CN, C$_2$H$_5$CN and CH$_2$=CH-CN in the temperature range 298–424 K. *Chem. Phys. Lett.* 80, 479–483.


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### 17.1 List of Chemicals and Data Compilations (by Functional Group)

**Aliphatic acids:**
- Dalapon

**Aromatic Acids:**
- Chloramben
- Dicamba
- Picloram

**Amides:**
- Alachlor
- Butachlor
- Diphenamid
- Metolachlor
- Napropamide
- Pronamide
- Propachlor
- Propanil

**Benzonitriles:**
- Bromoxynil
- Dichlobenil

**Carbamates:**
- Barban
- Chlorpropham
- Propham

**Dinitroanilines:**
- Benefin
- Butralin
- Dinitramine
- Fluchloralin
- Isopropalin
- Nitralin
- Oryzalin
- Pendimethalin
- Profuralin
- Trifluralin

**Diphenylethers:**
- Bifenox
- Fluorodifen
- Nitrofen

**Phenols:**
- Dinoseb

PCP (Pentachlorophenol) (See Chapter 14. Phenolic Compounds and Chapter 18. Insecticides)

**Phenoxyalkanoic acids:**
- 2,4-D
- 2,4-DB
- Dichlorprop
- Fenoprop
- MCPA
- MCBP
- Mecoprop
- 2,4,5-T

**Thiocarbamates:**
- Butylate
- Diallate
- EPTC
- Molinate
Ureas:
- Pebulate ................................................................. 3618
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- Ametryn ................................................................. 3466
- Atrazine ................................................................. 3471
- Chlorotoluron .......................................................... 3510
- Diuron ................................................................. 3551
- Fenuron ................................................................. 3562
- Fluometuron ............................................................ 3566
- Isoproturon .............................................................. 3577
- Linuron ................................................................. 3580
- Monolinuron ............................................................ 3600
- Monuron ................................................................. 3602
- Neburon ................................................................. 3608

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- Bromacil ................................................................. 3486
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- Chlorbromuron ........................................................ 3502
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- Chlorotoluron .......................................................... 3510
- Diuron ................................................................. 3551
- Fenuron ................................................................. 3562
- Fluometuron ............................................................ 3566
- Isoproturon .............................................................. 3577
- Linuron ................................................................. 3580
- Monolinuron ............................................................ 3600
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- Amitrole (Triazole). .................................................. 3469
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- Fluridone (Fluoro-phenyl pyridinone) ......................... 3569
- Glyphosate (Phosphate) ........................................... 3572
- Norflurazon ............................................................ 3614
- Pyrazon (Pyridazinone) ............................................ 3647
- Triclopyr (pyridine, organochlorine) ......................... 3668
17.1 LIST OF CHEMICALS AND DATA COMPILATIONS (By Functional Group)

17.1.1 HERBICIDES

17.1.1.1 Alachlor

Common Name: Alachlor
Synonym: alachlore, aloclor, Alanex, Bronco, Bullet, Cannon, Lasso, Lazo, metachlor, Pillarzo
Chemical Name: 2-chloro-2,6-diethyl-N-methoxymethylacetanilide; 2-chloro-N-(2,6-diethylphenyl)-N-(methoxy- methyl)acetamide
Uses: pre-emergence, early post-emergence or soil-incorporated herbicide to control most annual grasses and many annual broadleaf weeds in beans, corn, cotton, milo, peanuts, peas, soybeans, sunflower, and certain woody ornamentals.
CAS Registry No: 15972-60-8
Molecular Formula: C14H20ClNO2
Molecular Weight: 269.768
Melting Point (°C):
40 (Lide 2003)
Boiling Point (°C):
100 (at 0.02 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
135 (at 0.30 mmHg, Herbicide Handbook 1989; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
240.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₘₐₜ (kJ/mol):
29.288 (DSC method, Plato 1972)
Entropy of Fusion, ΔSₘₐₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₜ = 56 J/mol K), F: 0.713 (mp at 40°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
200 (Bailey & White 1965)
240 (Hartley & Graham-Bryce 1980; Beste & Humbug 1983)
148 (Khan 1980)
130 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
148, 242 (literature data variability, Heller et al. 1989)
140 (23°C, Budavari 1989)
240 (Wauchope 1989)
23.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)
140 (23°C, Milne 1995)
512 (predicted-AQUAFAC, Lee et al. 1996)
532, 785 (supercooled liquid S₂; literature derived value LDV, final adjust value FAV, Muir et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated):
- 0.00293 (20–25°C, Weber et al. 1980)
- 0.00293 (Ashton & Crafts 1981; Schnoor & McAvoy 1981; Schnoor 1992)
- 0.00290 (Beste & Humburg 1983)
- 0.00290 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 0.00300 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
- 0.00187 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.00413 (Montgomery 1993)
- 0.0064 (supercooled liquid P_L): literature derived value LDV, final adjust value FAV, Muir et al. 2004

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 6.20 × 10^{-3} (20°C, calculated-P/C, Suntio et al. 1988)
- 8.43 × 10^{-4} (wetted-wall-GC/ECD, Fendinger & Glotfelty 1988)
- 3.26 × 10^{-3} (calculated-P/C, Taylor & Glotfelty 1988)
- 1.12 × 10^{-3} (fog chamber-GC/ECD, Fendinger et al. 1989)
- 8.38 × 10^{-4} (23°C, known LWAPC of Fendinger et al. 1989, Meylan & Howard 1991)
- 1.21 × 10^{-5} (bond-estimated LWAPC, Meylan & Howard 1991)
- 3.26 × 10^{-3} (20°C, calculated-P/C, Muir 1991)
- 6.20 × 10^{-3} (calculated-P/C, Montgomery 1993)
- 3.22 × 10^{-3} (Gish et al. 1995)
- 7.24 × 10^{-3*} (Gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)

\[ \ln \left[ \frac{H'}{(M \text{ atm}^{-1})} \right] = -20.946 + \frac{9200}{(T/K)}; \text{ temp range } 283 \text{ to } 298 \text{ K} \] (gas stripping-GC/MS, Gautier et al. 2003)

0.00101. 1.49 (literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- 2.92 (Leo et al. 1971)
- 2.30 (Kenaga 1980)
- 2.64 (Rao & Davidson 1980)
- 3.087 (shake flask, Dubelman & Bremer 1983)
- 3.52 (shake flask, Log P Database, Hansch & Leo 1987)
- 3.27 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 3.52 (recommended, Sangster 1993)
- 3.52 (recommended, Hansch et al. 1995)
- 3.27 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 3.09 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log \( K_{OA} \):
- 9.31 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
- 1.45 (calculated-solubility, Kenaga 1980)
- 0.954 (calculated-\( K_{OC} \), Kenaga 1980)
- 1.88 (Schnoor & McAvoy 1981, Schnoor 1992)
- 0.778 (freshwater fish, Cali et al. 1984)
- 1.70 (Pait et al. 1992)

Sorption Partition Coefficient, log \( K_{OC} \):
- 2.28 (soil, Beestman & Demming 1976)
- 2.32 (soil, calculated, Kenaga & Goring 1980)
- 2.30 (soil, Kenaga 1980)
- 1.70 (sediment/water, Schnoor & McAvoy 1981)
1.91 (soil, average for soils 2–7, Weber & Peter 1982)
2.08 (soil, screening model calculations, Jury et al. 1987b)
2.28 (Carsel 1989)
2.18, 2.23, 2.28, 2.53 (soil, lit. values, Bottoni & Funari 1992)
1.63–2.28 (quoted values, Montgomery 1993)
2.21 (selected, Wienhold & Gish 1994)
2.28 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.28; 2.53 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.22, 2.22, 2.20 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

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

Volatileization: k(measured) = 9000 d⁻¹ and k(estimated) = 49000 d⁻¹ (Glotfelty et al. 1989);
estimated t½ = 2444 d from 1-m depth of water at 20°C (Muir 1991)
Volatilization rate k = 4.4 × 10⁻⁴ d⁻¹, 2.8 × 10⁻³ d⁻¹, 4.3 × 10⁻³ d⁻¹ at 15, 25, 35°C, respectively, for commercial
formulation; k = 5.8 × 10⁻⁵ d⁻¹, 8.7 × 10⁻⁵ d⁻¹, 1.4 × 10⁻² d⁻¹ at 15, 25, 35°C, respectively, for starch
encapsulated formulation after application (Weinhold et al. 1993)

Photolysis: t½ = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991); 640 ppb contaminated
water in the presence of TiO₂ and H₂O₂ photodegraded to 3.5 ppb by 15 h solar irradiation with complete
degradation after 75 h (Muszkat et al. 1992).

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:
k(aq.) = (3.8 ± 0.4) M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 2–6.0 and 21°C, with a half-life
of 2.4 h at pH 7 (Yao & Haag 1991).
k(calc) = 7 × 10⁶ M⁻¹ s⁻¹ for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao
1992) kOH = 2.3 × 10⁻¹⁰ cm³·molecule⁻¹ s⁻¹ with calculated tropospheric lifetime about 0.5 d at 298 K
assuming an average OH concn of 1 × 10⁶ molecule/cm³ (Gautier et al. 2003)


Biodegradation: t½ < 6 months for 0.07 µg/mL to biodegrade in groundwater, t½ > 15 months for 10.0 µg/mL
to biodegrade in ground water both at 25°C and t½ < 12 wk for 3.2 µg/mL to biodegrade in soil-water
suspension at 35°C (Weidner 1974; quoted, Muir 1991);
t½ = 23 d for 0.244 µg/mL to biodegrade in river water at 23°C with biodegradation rate k = 0.030 d⁻¹
(Schnoor et al. 1982; quoted, Muir 1991);
t½ = 18 d from screening model calculations (Jury et al. 1987b);
t½ > 6 wk for 0.01–1.0 µg/mL to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander
1985; quoted, Muir 1991);
overall degradation rate constant k = 0.0403 h⁻¹ with t½ = 17.2 h in sewage sludge and rate constant
k = 0.1601 d⁻¹ with t½ = 4.3 d in garden soil (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime of 0.5 d for gas phase reaction with OH radicals; wet deposition lifetime estimated to
be 2.8 d in the atmosphere by rainfall (Gautier et al. 2003)
Surface water: t½ = 23 d for 0.244 µg/mL to biodegrade in river water at 23°C with biodegradation rate k = 0.030 d⁻¹
(Schnoor et al. 1982; quoted, Muir 1991);
t½ > 6 wk for 0.01–1.0 µg/ml to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander
1985; quoted, Muir 1991);
k(measured) = (3.8 ± 0.4) M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 2–6 and 21°C, with t½ = 2.4 h
at pH 7 (Yao & Haag 1991).

Ground water: t½ < 6 months for 0.07 µg/mL to biodegrade in groundwater, and t½ > 15 months for 10.0 µg/mL
to biodegrade in groundwater both at 25°C (Weidner 1974; quoted, Muir 1991) reported t½ = 7, 4–21 and
38 d (Bottoni & Funari 1992)

Sediment:
Soil: dissipation $t_{1/2} = 7.8$ d in soil (Beestman & Demming 1974); measured dissipation rate $k = 0.077$ d$^{-1}$ (Zimdahl & Clark 1982);
$t_{1/2} = 23$ and 5.7 d in soil containing 6 and 15% moisture, respectively (Walker & Brown 1985);
$t_{1/2} = 18$ d from screening model calculations (Jury et al. 1987b);
estimated dissipation rate $k = 0.020$ and 0.036 d$^{-1}$ (Nash 1988);
field $t_{1/2} < 1.5$ wk by using field lysimeters (Bowman 1990);
degradation rate constant $k = (4.52 \pm 0.192) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 15.3$ d in control soil and $k = (7.27 \pm 0.772 \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 9.53$ d in pretreated soil in the field; $k = (2.77 \pm 0.226) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 25$ d in control soil and $k = (14.1 \pm 1.75) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 4.93$ d in pretreated soil once only in the laboratory (Walker & Welch 1991);
selected field $t_{1/2} = 15$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Richards & Baker 1993);
soil $t_{1/2} = 30$ d (quoted, Pait et al. 1992);
reported $t_{1/2} = 7$, 4–21 and 38 d (Bottoni & Funari 1992);
soil $t_{1/2} = 14–28$ d (Di Guardo et al. 1994);
dissipation $t_{1/2} = 42$ d from soil surface (Gish et al. 1995);
degradation $t_{1/2} = 4.3$ d in garden soil (Müller & Buser 1995);
$t_{1/2} = 15$ d (selected, Halfon et al. 1996);
dissipation $t_{1/2}(\text{calc}) = 5$ and 5.3 d in soil in model ecosystem, $t_{1/2} = 3.3$ and 3.4 d in water in model ecosystem (Ramesh & Maheswari 2004).

Biota: biochemical $t_{1/2} = 18$ d from screening model calculations (Jury et al. 1987b).

**TABLE 17.1.1.1.1**
Reported Henry’s law constants of alachlor at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$H/(\text{Pa m}^3/\text{mol})$</th>
<th>$t/°C$</th>
<th>$H/(\text{Pa m}^3/\text{mol})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$1.097 \times 10^{-3}$</td>
<td>10</td>
<td>$1.26 \times 10^{-3}$</td>
</tr>
<tr>
<td>10</td>
<td>$1.30 \times 10^{-3}$</td>
<td>10</td>
<td>$9.76 \times 10^{-4}$</td>
</tr>
<tr>
<td>11</td>
<td>$2.115 \times 10^{-3}$</td>
<td>15</td>
<td>$1.68 \times 10^{-3}$</td>
</tr>
<tr>
<td>12</td>
<td></td>
<td>17</td>
<td>$2.58 \times 10^{-3}$</td>
</tr>
<tr>
<td>18</td>
<td>$3.13 \times 10^{-3}$</td>
<td>20</td>
<td>$4.24 \times 10^{-3}$</td>
</tr>
<tr>
<td>23</td>
<td>$3.07 \times 10^{-3}$</td>
<td>23</td>
<td>$3.07 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Arrhenius expression:

$$\ln H'/(\text{M atm}^{-1}) = -A + B/(T/K)$$

$A = 20.946$, $B = 9200$.
FIGURE 17.1.1.1 Logarithm of Henry’s law constant versus reciprocal temperature for alachlor.
17.1.1.2 Ametryn

Common Name: Ametryn
Synonym: Amephyt, Ametrex, Evik, Gesapax
Chemical Name: 6-methylthio-2-(ethylamino)-4-(isopropylamino)-1,3,5-triazine; N-ethyl-N′-(1-methylethyl)-6-(methyl-thio)-1,3,5-triazine-2,4-diamine
Uses: herbicide to control broadleaf and grass weeds in corn, sugarcane, some citrus fruits, and in noncropland; also used as pre-harvest and post-harvest dessicant in potatoes to control crop and weeds.

CAS Registry No: 834-12-8
Molecular Formula: C₉H₁₇N₅S
Molecular Weight: 227.330
Melting Point (°C): 88 (Lide 2003)
Boiling Point (°C): 328.78 (Rordorf 1989)
Density (g/cm³ at 20°C): 1.19 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Molar Volume (cm³/mol): 277.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
- 4.00 (pKₐ, Weber 1970; quoted, Bintein & Devillers 1994)
- 4.10 (pKₐ, Worthing & Hance 1991; Montgomery 1993)
- 9.90 (pKₐ, Tomlin 1994)

Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
91.96 (Rordorf 1989)
Enthalpy of Fusion, ∆Hₕus (kJ/mol):
19.8 (Rordorf 1989)
Entropy of Fusion, ∆Sₕus (J/mol K):
55 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ∆Sₕus = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 700 (Woodford & Evans 1963)
- 405, 195, 192 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
- 185 (Martin & Worthing 1977; Herbicide Handbook 1978)
- 194 (Weber et al. 1980)
- 200 (Tomlin 1994)
- 134 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.12 × 10⁻⁴ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964) (See figure at the end of this section.)
1.12 × 10⁻⁴ (20°C, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)

log (P_s/kPa) = 11.036 – 5270/(T/K), temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
1.00 × 10⁻⁴ (20°C, selected, Suntio et al. 1988)
3.74 × 10⁻⁴, 1.40 × 10⁻², 0.30, 4.40, 46 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P_s/Pa) = 16.85 – 6048.6/(T/K); measured range 49.5–85°C (gas saturation-GC, Rordorf 1989)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.20 × 10⁻⁴ (20°C, calculated, Suntio et al. 1988)
1.38 × 10⁻⁴ (calculated-P/C, Montgomery 1993)
1.23 × 10⁻⁴ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:
2.69 (Kenaga & Goring 1980)
2.58 (Gerstl & Helling 1987)
2.98 (shake flask, Log P Database, Hansch & Leo 1987)
2.82 (Worthing & Hance 1991)
2.98 (shake flask, Biagi et al. 1991)
3.07 (RP-HPLC-RT correlation, Finizio et al. 1991)
2.88 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.98 (recommended, Sangster 1993)
2.63 (Tomlin 1994)
2.61 (shake flask-UV, Liu & Qian 1995)
2.58 (calculated-RP-HPLC-k’ correlation, Liu & Qian 1995)
2.83 (Milne 1995)
2.98 (recommended, Hansch et al. 1995)
2.88 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.52 (calculated-S, Kenaga 1980)
1.32 (calculated-K_{oc}, Kenaga 1980)

Sorption Partition Coefficient, log K_{oc}:
2.59 (soil, Hamaker & Thompson 1972;)
2.40 (soil, calculated, Kenaga & Goring 1980)
2.59 (soil, Kenaga & Goring 1980)
2.59 (Rao & Davidson 1980)
2.59, 2.86 (quoted, calculated-MCI_χ, Gerstl & Helling 1987)
2.59, 2.51 (reported as log K_{om}, estimated as log K_{om}, Magee 1991)
2.40–2.59, 2.58 (soil, quoted values, Bottoni & Funari 1992)
2.23–2.44 (Montgomery 1993)
2.48 (Tomlin 1994)
2.42 (calculated-K_{oc}, Liu & Qian 1995)
2.59 (soil, calculated-MCI_χ, Sabljic et al. 1995)
2.70, 2.59 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.52, 2.63, 2.60, 2.35 (soils with organic carbon OC ≥ 0.5% at: pH 4.5–9.0, pH 4.5–5.4, pH 5.5–6.0, pH-6.1, average, Delle Site 2001)
1.84, 2.23 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{\text{hal}}$:

Volatilization:
- Photolysis: $t_{\text{hal}} = 10$ h for 10 $\mu$g mL$^{-1}$ to degrade in distilled water under > 290 nm light and $t_{\text{hal}} = 3.3$ h in 1% acetone solution (Burkhard & Guth 1976; quoted, Cessna & Muir 1991);
- $t_{\text{hal}} = 2.25$ h for 17% of 33 $\mu$g mL$^{-1}$ to degrade in 0.2% aqueous solutions of the surfactant Triton X-100 and for 8% of 33 $\mu$g/mL to degrade in distilled water both under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:
- Hydrolysis: $t_{\text{hal}} = 32$ d at pH 1 and $t_{\text{hal}} > 200$ d at pH 13 (Montgomery 1993).

Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater: reported half-lives or persistence, $t_{\text{hal}} = 7$–120 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{\text{hal}} = 6.0$ months at 15°C and $t_{\text{hal}} = 4.5$ months at 30°C in soils (Freed & Haque 1973);
- $t_{\text{hal}} = 70$–120 d (Bottoni & Funari 1992);
- selected $t_{\text{hal}} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);
- $t_{\text{hal}} = 70$–129 d in soil (Tomlin 1994).

Biota:

![Ametryn: vapor pressure vs. 1/T](image)

**FIGURE 17.1.2.1** Logarithm of vapor pressure versus reciprocal temperature for ametryn.
17.1.1.3 Amitrole

Common Name: Amitrole
Synonym: Amazole, Amitrol, Amizole, aminotriazole, Azolan, Azole, cytrol, Diurol
Chemical Name: 3-amino-1,2,4-triazole; 3-amino-s-triazole; 1H-1,2,4-triazol-3-amine
Uses: nonselective, foliage-applied herbicide in uncropped land and orchards to control perennial weeds in certain grasses.
CAS Registry No: 61-82-5
Molecular Formula: C₂H₄N₄
Molecular Weight: 84.080
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   85.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘ (kJ/mol):
   24.69  (DSC method, Plato 1972)
Entropy of Fusion, ∆Sₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₘ = 56 J/mol K), F: 0.0484 (mp at 159°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   252000  (Freed & Burschel 1957)
   280000  (Martin 1961; Spencer 1981)
   soluble  (Wauchope 1978)
   280000  (20°C at pH 7, quoted, Montgomery 1993)
   280000  (23°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
   < 0.001  (Agrochemicals Handbook 1983; quoted, Howard 1991)
   < 0.001  (Hartley & Kidd 1987)
   5.50 × 10⁻⁸ (20°C, Worthing & Hance 1991; Tomlin 1994)
   5.51 × 10⁻⁷ (20°C, quoted, Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
   < 3.04 × 10⁻⁷  (calculated-P/C, Howard 1991)
   1.650 × 10⁻¹₀  (20°C, calculated-P/C, Montgomery 1993)
   1.650 × 10⁻¹₀  (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{ow}$:
- 0.85 (shake flask, pH 7, Lichtner 1983)
- 0.52 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 0.15 (Reinert 1989; quoted, Howard 1991; Montgomery 1993)
- 0.87, –0.84 (pH 7) (Hansch et al. 1995)
- 0.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
- 0.301 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)
- 0.347 (estimated-log $K_{ow}$, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log $K_{oc}$:
2.04 (soil, estimated-molecular topology & QSAR, Sabljic 1984)
0.23 (calculated-MCI $\chi$, Gerstl & & Helling 1987)
1.26 (Reinert 1989)
2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.73–2.31 (quoted, Montgomery 1993)
2.00 (estimated-chemical structure, Lohninger 1994)
1.25 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2} = 3.2–32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis:
Biodegradation: aqueous aerobic $t_{1/2} = 672–4032$ h, based on reported half-lives in soil and water (Freed & Haque 1973; Reinert & Rogers 1987; 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:

Half-Lives in the Environment:
Air: $t_{1/2} = 3.8$ d, based on a theoretical calculation for the vapor-phase reaction with hydroxyl radicals in the atmosphere at 25°C (GEMS 1986; quoted, Howard 1989); $t_{1/2} = 3.2–32$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Groundwater: $t_{1/2} = 1344–8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1/2} = 1.4, 1.6, 1.3, 92, 36, and 56$ d with disappearance rates: $k = 0.495, 0.433, 0.533, 0.0075, 0.0193$, and $0.124$ d$^{-1}$ at pH 6.0, 7.0, 8.0, 5.3, 6.5, and 7.5 (Hamaker 1972; quoted, Nash 1988); $t_{1/2} = 1.5$ month at 15°C and $t_{1/2} = 1.0$ month at 30°C in soils (Freed & Haque 1973); persistence of one month in soil (Wauchope 1978); persistence in soil for ca. 2–4 wk (Herbicide Handbook 1989; Tomlin 1994); $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); selected field $t_{1/2} = 14$ d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:
17.1.1.4 Atrazine

Common Name: Atrazine
Chemical Name: 2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine; 6-chloro-N-ethyl-N’-(1-methylethyl)-1,3,5-triazine-diamine
Uses: pre-emergence and post-emergence herbicide to control some annual grasses and broadleaf weeds in corn, fallow land, rangeland, sorghum, noncropland, certain tropical plantations, evergreen nurseries, fruit crops, and lawns.
CAS Registry No: 1912-24-9
Molecular Formula: C₈H₁₄ClN₅
Molecular Weight: 215.684
Melting Point (°C): 173 (Lide 2003)
Molar Volume (cm³/mol): 250.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
- 1.68 (pKₐ, Weber 1970; Somasundaram et al. 1991; Bintein & Devillers 1994)
- 1.60 (pKₐ, Yao & Haag 1991; Haag & Yao 1992)
- 1.62 (pKₐ, 20°C, Montgomery 1993)
Enthalpy of Fusion, ΔHₐus (kJ/mol):
- 40.585 (DSC method, Plato 1972)
Entropy of Fusion, ΔSₐus (J/mol K):
- Fugacity Ratio at 20°C (assuming ΔSₐus = 56 J/mol K), F: 0.0353 (mp at 173°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 70.0 (26°C, Bailey & White 1965)
- 50.0 (Günther et al. 1968)
- 31.1, 34.9, 36.8 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
- 98.0 (50°C, Getzen & Ward 1971)
- 33.0 (shake flask-GC, Hörmann & Eberle 1972)
- 29.9 (shake flask-UV, Hurle & Freed 1972)
- 32.0 (Freed 1976; Beste & Humburg 1983; Jury et al. 1983)
- 31.5 (Spencer 1976)
- 33.0 (Wauchope 1978; Kenaga 1980; Kenaga & Goring 1980)
- 35.0 (Weber et al. 1980)
- 30.0 (shake flask-HPLC, Ellgehausen et al. 1981)
- 24.0 (Thomas 1982)
- 70.0 (Windholz 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):

44.0 × 10⁻⁵* (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964)

log (P/mmHg) = 13.766 – 5945/(T/K), temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)


3.99 × 10⁻⁵ (20°C, gas saturation, extrapolated from Friedrich & Stammbach 1964, Spencer 1976)

4.00 × 10⁻⁵ (20°C, Hartley & Graham-Bryce 1980; Beste & Humbug 1983)

4.00 × 10⁻⁵ (20–25°C, Weber et al. 1980)

4.00 × 10⁻⁵ (20°C, Ashton & Crafts 1981)

1.33 × 10⁻⁴ (selected, Schnoor & McAvoy 1981)

3.70 × 10⁻⁵ (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)

\ln (P/Pa) = 36.8 – 13778/(T/K), for temp range 51–81.5°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)

1.13 × 10⁻⁴ (Thomas 1982)

4.00 × 10⁻⁵ (20°C, Hartley & Kidd 1987)

\log (P_Pa/kPa) = 12.8909 – 59450/(T/K), temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)

8.70 × 10⁻⁵ (selected, Nash 1989)


3.90 × 10⁻⁵ (gas saturation-GC, measured range 40.5–125°C, Rordorf 1989)

log (P_Pa) = 13.27071 – 6558.5/(T/K); measured range not specified (gas saturation-GC, Rordorf 1989)

4.05 × 10⁻⁵ (Riederer 1990)


4.00 × 10⁻⁵ (20°C, Montgomery 1993)

2.00 × 10⁻⁵ (selected, Sieber et al. 1994)

3.90 × 10⁻⁵ (Tomlin 1994; quoted, Halfon et al. 1996)


log (P/Pa) = 16.08 – 6040/(T/K); temp range 40–80°C, Goodman 1997)

0.0096, 0.0096 (supercooled liquid P_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):


2.90 × 10⁻⁴ (20°C, calculated-P/C, Suntio et al. 1988)

6.19 × 10⁻⁴ (calculated-P/C, Taylor & Glotfelty 1988)

5.70 × 10⁻⁴ (calculated-P/C, Nash 1989)

3.04 × 10⁻⁴ (Riederer 1990)

2.66 × 10⁻⁴ (calculated-P/C, Howard 1991)

2.89 × 10⁻⁴ (20°C, calculated-P/C, Muir 1991)

3.08 × 10⁻⁴ (20°C, calculated-P/C, Montgomery 1993)

1.00 × 10⁻³ (calculated-P/C, Sieber et al. 1994)

6.20 × 10⁻⁴ (Gish et al. 1995)

2.88 × 10⁻⁴ (calculated-P/C, this work)

0.518 (final adjust value FAV, Muir et al. 2004)
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Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.75 (shake flask-GC, Erkell & Walum 1979)
- 2.63 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1982)
- 2.35 (Rao & Davidson 1980)
- 2.71 (shake flask-both phases analyzed by GC and UV spec., Brown & Flagg 1981)
- 2.40, 2.21 (HPLC-$k'$ correlation, McDuffie 1981)
- 2.75 (shake flask, Ellgehausen et al. 1981)
- 2.80 (Elgar 1983)
- 2.05 (RP-HPLC-$k'$ correlation, Braumann et al. 1983)
- 2.64 (shake flask-GC, Geyer et al. 1984)
- 2.75 (Hansch & Leo 1985)
- 2.64 (OECD method 1981, Kerler & Schönherr 1988)
- 2.68 (Lopez-Avila et al. 1989)
- 2.61, 2.61 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.34 (Worthing & Hance 1991; Milne 1995)
- 2.10 (shake flask, pH 7, Baker et al. 1992)
- 2.33–2.80 (quoted values, Montgomery 1993)
- 2.75 (recommended, Sangster 1993)
- 2.42 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.50 (Tomlin 1994)
- 2.27 (shake flask-UV, Liu & Qian 1995)
- 2.61 (selected, Hansch et al. 1995)
- 2.43 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 2.00 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
- 2.63 ± 0.07, 2.47 ± 0.15, 2.46 ± 0.09 (shake flask, isocratic RP-HPLC-$k'$ correlation, gradient RP-HPLC-$k'$ correlation, Paschke et al. 2004)
- 2.40 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log $K_{OA}$:
- 9.08 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
- $< 2.00$ (vegetation, correlated-$K_{OW}$, Beynon et al. 1972; quoted, Travis & Arms 1988)
- 1.04 (Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 1.00 (Isensee 1976)
- 0.50 (whitefish, Burkhard & Guth 1976)
- 0.90 (fathead minnow, Veith et al. 1979)
- 0.30 (catfish, Ellgehausen et al. 1980; quoted, Howard 1991)
- 0.26 ($Daphnia magna$, wet wt. basis, Ellgehausen et al. 1980)
- 0.48 ($Corygonus fera.$ at 12°C, Gunkel & Streit 1980)
- 1.93, 0.845 (calculated-S, $K_{OW}$, Kenaga 1980)
- $< 0.90$ (Veith et al. 1980)
- 1.90 (selected, Schnoor & Mcavoy 1981)
- 1.93, 1.77 (estimated-S, estimated-$K_{OW}$, Bysshe 1982)
- 0.90 (fathead minnow, Veith & Kosian 1982)
- 2.00 (mottled sculpin, Lynch et al. 1982)
- 1.60 (activated sludge, Freitag et al. 1984)
- 1.00 (golden ide, Freitag et al. 1985)
- 0.477, 0.845, 0.778 (zebrafish: egg, embryo, yolk sac fry, juvenile; Gorge & Nagel 1990)
- 0.78 ($Brachydanio rerio$, Gorge & Nagel 1990)
- 0.983 ($Hydrilla$, Himnan & Klaine 1992)
- 1.98, 0.748, 0.230 (algae $Scenedesmus acutus$, catfish $Ictalurus melas$, $Daphnia magna$, wet wt. basis, Wang et al. 1996)
### Bioaccumulation Factor, log BAF:

- 1.710 (algae, Ellgehausen et al. 1980)
- 0.329 (catfish, Ellgehausen et al. 1980)
- 0.261 (daphnids, Ellgehausen et al. 1980)
- 1.72, 0.477, 1.60 (algae, fish, sludge, Klein et al. 1984)
- 1.70, < 1.00, 1.60 (algae, fish, sludge, Freitag et al. 1985)

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

- 2.17 (soil, Hamaker & Thompson 1972)
- 2.09 (average of 4 soils, Rao & Davidson 1979; Davidson et al. 1980)
- 2.81 (calculated, Kenaga & Goring 1980; Kenaga 1980)
- 2.20 (average of soils/sediments, Rao & Davidson 1980)
- 2.21 (average of 56 soils from lit. review, Rao & Davidson 1980)
- 2.33 (a Georgia pond sediment, sorption isotherms by shake flask-GC/ECD, Brown & Flagg 1981)
- 1.59 (a Swiss soil, Burkhard & Guth 1981)
- 3.11, 2.31; 1.94, 2.42 (estimated-S, calculated-S and mp; estimated-$K_{OM}$, Karickhoff 1981)
- 0.7–1.48 (selected, sediment/water, Schnoor & McAvoy 1981)
- 2.18 (soil, Thomas 1982)
- 2.29–3.18 (Wolf & Jackson 1982)
- 3.23–4.13 (Means & Wijayaratne 1982)
- 2.21 (soil average, Jury et al. 1983)
- 1.63–3.29 (Wauchope & Myers 1985; 1991)
- 2.46 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 2.20 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.92 (RP-HPLC-k’ correlation, cyanopropyl column, Hodson & Williams 1988)
- 2.21 (estimated as log $K_{OM}$, Magee 1991)

- 2.0, 2.18, 2.17–2.81, 2.26 (soil, literature values, Bottoni & Funari 1992)
- 2.27, 2.41, 2.59, 2.16 (soils, no. 1, 2, 3, 4; Francioso et al. 1992)
- 1.81 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 1.95–2.71 (quoted values, Montgomery 1993)
- 2.60 (soil with 9.23% organic carbon, Donati et al. 1994)
- 2.04 (agricultural soil, Douset et al. 1994)
- 2.40 (estimated-chemical structure, Lohninger 1994)
- 2.05 (soil with low organic carbon 0.18%, Roy & Krapac 1994)
- 1.95–2.19 (Tomlin 1994)
- 2.23 (calculated-$K_{OM}$, Liu & Qian 1995)
- 2.24 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.81; 2.36 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.00 (sediment/water, Chung et al. 1996)
- 2.64 (Levy wetland soil, sorption equilibrium technique, 24°C, Mersie & Seybold 1996)
- 2.14–2.21; 2.03–2.12 (Teufelsweiher pond sediment: field measurement; exp. laboratory data, Gao et al. 1997)
- 2.19 (sediment from Teufelsweiher pond, batch equilibrium isotherm, Gao et al. 1998)
- 1.93, 1.80–1.85, 1.81 (soil, liquid sewage sludge amended soil, sludge, pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 1.93, 1.83, 1.79 (soil + CaCl$_2$ at pH 7.2, soil + liquid sewage sludge and dissolved organic matter at pH 7.5, soil + liquid sewage sludge at pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 2.566, 1.72, 1.75, 1.505, 2.40 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.24, 2.45; 2.82, 1.81, 2.81, 1.98, 1.99 (quoted lit., calculated-$K_{OM}$, HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.154, 1.97, 1.77, 1.61, 2.496 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
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1.69  (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
2.154, 1.969, 1.769, 1.610, 2.486 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
2.24; 2.27, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.59, 2.16 (average values for sediments, soils, Delle Site 2001)
2.59, 2.16 (average values for sediments, soils, Delle Site 2001)
2.31, 2.17, 2.56 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 3.2–8.2, average, Delle Site 2001)
2.34, 2.24, 2.06, 2.59 (soils with organic carbon OC ≥ 0.5% at: pH 3.2–5.0, pH 5.1–5.9, pH 6.0, pH 4.4–7.7, average, Delle Site 2001)
1.77, 2.10  (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: initial rate constant k = 6.4 × 10–4 h–1 and predicted rate constant k = 4.2 × 10–4 h–1 from soil with t½ = 1650 h (Thomas 1982);
t½ = 97 d (Jury et al. 1983; quoted, Grover 1991);
rate constants k(measured) = 1100 d–1 and k(est.) = 6000 d–1 (Glotfelty et al. 1989);
Half-lives from soil surfaces: t½ = 655 to > 1000 d in peat soil and t½ = 143–939 d in sandy soil; half-lives from plant surfaces: t½ = 25.6 d in bean, t½ = 24.3 d in turnips and t½ = 14.6 d in oats at 20 ± 1°C (Dörfler et al. 1991)
Volatilization rate k = 1.4 × 10–4 d–1, 2.6 × 10–4 d–1, 4.4 × 10–4 d–1 at 15, 25, 35°C, respectively, for commercial formulation; k = 1.2 × 10–5 d–1, 4.8 × 10–4 d–1, 8.1 × 10–4 d–1 at 15, 25, 35°C, respectively, for starch-encapsulated formulation after application (Weinhold et al. 1993)
Photolysis: t½ = (19 ± 9) h under summer sunlight of 9.1 h d–1 exposure and t½ = 61 ± 9 h under spring sunlight of 3.7 h d–1 exposure in 10 ppm aqueous solutions: (Burkhard et al. 1975);
t½ = 4.9 h for 10 µg/mL to degrade in 1% acetone solution and t½ = 25 h for 10 µg/mL to degrade in distilled water both under > 290 nm light (Burkhard & Guth 1976);
nearsurface direct sunlight photolysis rate constant k = 9 × 10–6 d–1 with t½ = 81,000 d (Schnoor & McAvoy 1981; quoted, Schnoor 1992);
t½ = 2.25 h for 17–27% of 100 µg/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
rate of photolytic degradation was slightly higher in water (t½ = 3–12 d) than in sediments (t½ = 1–4 wk) (Jones et al. 1982; quoted, Montgomery 1993);
40 ppb contaminated water in presence of TiO2 and H2O2 degraded to 4 ppb after 15 h by solar irradiation with complete degradation after 75 h (Muszkat et al. 1992)

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 = 147.2 × 10–12 cm3 molecule–1 s–1 with h half-life of 2.6 h at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
k(aq.) = 5.9 × 109 M–1 s–1 for the reaction (photo-Fenton with reference to acetophenone) with OH radical in aqueous solutions at pH 3.6 and 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
k(aq.) = (24 ± 4) M–1 s–1 for direct reaction with ozone at pH 4 and 26°C; k = (13 ± 1) M–1 s–1 at pH 4.2 and 21°C and k = (24 ± 4) M–1 s–1 at pH 4.1 and 19°C in water, with a half-life of 1.5 h at pH 7 (Yao & Haag 1991)
k(aq.) = (2.6 ± 0.4) × 109 M–1 s–1 for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.6 and 24 ± 1°C (Haag & Yao 1992)
k(aq.) = 0.82 × 109 M–1 s–1 for reaction with hydroxyl radical in irradiated field water (Mabury & Crosby 1996)
Hydrolysis: $t_{1/2} \approx 70$ d at pH 3.1 of citrate buffer; $t_{1/2} \approx 75$ d at pH 11.1 of carbonate buffer and $t_{1/2} \approx 2$ d at 3.9 of phosphate buffer + sterile lake sediment in aqueous solutions at 25°C (Armstrong et al. 1967; quoted, Muir 1991)

Over all rate constant $k = 7.6 \times 10^{-5}$ s$^{-1}$ with $t_{1/2} = 2.5$ h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 3.3, 14, 58, 240, 100, 12.5, and 1.5$ d at pH 1, 2, 3, 4, 11, 12, and 13, respectively, in aqueous buffered solutions in soil at 25°C (Armstrong et al. 1967; quoted, Montgomery 1993); $t_{1/2} = 244$ d without humic materials, $t_{1/2} = 1.37$ d with the presence of 2% humic acid at pH 4 and 25°C (Li & Felbeck 1972; quoted, Howard 1991; Montgomery 1993)

$k = 3.9 \times 10^{-5}$ M$^{-1}$ s$^{-1}$ and $k = 7.6 \times 10^{-5}$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 66$ and 81 d in aqueous solutions of pH 3.1 and 11.1, respectively (Wolfe et al. 1976; quoted, Muir 1991)

$k(aq.) = 19.9$ d$^{-1}$ at pH 2.9, $k = 3.99$ d$^{-1}$ at pH 4.5, $k = 1.74$ d$^{-1}$ at pH 6.0, and $k = 0.934$ d$^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 34.8, 174, 398,$ and 742 d all at 25°C in 0.5 mg mL$^{-1}$ concn. of aqueous fulvic acid (Khan 1978; quoted, Howard 1991; Montgomery 1993)

$k(aq.) = 28.4$ d$^{-1}$ at pH 2.8, $k = 12.6$ d$^{-1}$ at pH 4.5, $k = 3.16$ d$^{-1}$ at pH 6.0, and $k = 1.23$ d$^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 24.4, 55.0, 219,$ and 563 d all at 25°C in 1.0 mg mL$^{-1}$ concn. of aqueous fulvic acid (Khan 1978)

$k(aq.) = 151$ d$^{-1}$ at pH 2.4, $k = 43.7$ d$^{-1}$ at pH 4.5, $k = 13.2$ d$^{-1}$ at pH 6.0, and $k = 7.93$ d$^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 4.60, 15.9, 52.5$ and 87.3 d all at 25°C in 5.0 mg mL$^{-1}$ concn. of aqueous fulvic acid (Khan 1978)

$k(aq.) = 9.30 \times 10^{-6}$ s$^{-1}$ with $t_{1/2} = 86$ d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981; quoted, Muir 1991)

$t_{1/2} > 3$ months (in sterile buffer solution at pH 7.2) and $t_{1/2} > 14$ d (in sterile mineral salt solution at pH 7.2) for 20 µg mL$^{-1}$ to hydrolyze at 23°C (Geller 1980; quoted, Muir 1991)

$k(alkaline) = 1 \times 10^{-16}$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 742$ d (Schnoor & McAvoy 1981; quoted, Schnoor 1992)

$t_{1/2} = 1771$ yr at pH 7 and 25°C (Montgomery 1993)

Biodegradation:

$t_{1/2} = 64$ d in soil (Armstrong et al. 1967; Dao et al. 1979; quoted, Means et al. 1983)

$t_{1/2} = 3.21$ d in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982)

$t_{1/2(aerobic)} > 90$ d for 10–20 µg mL$^{-1}$ to degrade in soil-water suspension (Goswami & Green 1971; quoted, Muir 1991)

$k(aq.) = 0.019$ d$^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2(aerobic)} > 35$ d for 0.1–1.0 µg mL$^{-1}$ to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2} = 36$ and 110 d in soil (Jones et al. 1982; quoted, Means et al. 1983)

$t_{1/2} = 71$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989; quoted, Grover 1991)

$k = 0.22$ d$^{-1}$ of aerobic degradation rate observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1995)

$t_{1/2} = 201$ d with 12 mM methanol, for aqueous atrazine using first-order decay rate, $t_{1/2} = 289$ d with 6 mM sodium acetate, $t_{1/2} = 164$ d with 6 mM acetic acid and $t_{1/2} = 200$ d with 2 mM glucose; however $t_{1/2} = 224$ d in the sample reactors without any organic amendments (Chung et al. 1996)

degradation $t_{1/2} = 39$ h and 43 h by soil micro Rhodococcus. sp. NI86/21 with atrazine concn 4 µg/mL and 8 µg/mL respectively (Van Zwieten & Kennedy 1995)

first order removal of atrazine from sediment organic carbon: $k = -0.0054$ d$^{-1}$ with $t_{1/2} = 128$ d in surface sediment 0–6 cm depth, $k = -0.0016$ d$^{-1}$ with $t_{1/2} = 433$ d in sub-surface sediment 24–34 cm depth from Blue Heron Pond; $k = -0.007$ d$^{-1}$ with $t_{1/2} = 99$ d in surface sediment 0–6 cm depth, $k = -0.0022$ d$^{-1}$ with $t_{1/2} = 630$ d in sub-surface sediment 24–34 cm depth from Oyster Rake Pond; $k = -0.0142$ d$^{-1}$ with $t_{1/2} = 49$ d in surface sediment 0–6 cm depth, $k = -0.0099$ d$^{-1}$ with $t_{1/2} = 770$ d in sub-surface sediment 24–34 cm depth from Trumpet Creeper East Pond, and $k = -0.0149$ d$^{-1}$ with $t_{1/2} = 47$ d in surface sediment 0–6 cm depth, $k = -0.0000$ d$^{-1}$ with $t_{1/2} = 70$ d in sub-surface sediment 24–34 cm depth from Trumpet Creeper North, Kiawah island (Smalling & Aelion 2004)

50–60% degradation in 35–100 d by anaerobic mixed culture microorganisms with atrazine as sole carbon source (Ghosh & Philip 2004)

Biotransformation:

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

\[ k_2 = 0.0248, \ 1.26 \ h^{-1} \] (algae, daphnids, Ellgehausen et al. 1980)
\[ k_2 = 27.2 \ d^{-1} \] (catfish, Ellgehausen et al. 1980)
\[ k_1 = 2.4, \ 30, \ 19.0 \ h^{-1} \] (zebrafish: egg, yolk sac fry, juvenile; Görge & Nagel 1990)
\[ k_1 = 227.0 \ h^{-1}; \ k_2 = 2.354 \ h^{-1} \] (algae Scenedesmus acutus, Wang et al. 1996)
\[ k_1 = 0.412 \ h^{-1}; \ k_2 = 0.073 \ h^{-1} \] (catfish Ictalurus melas, Wang et al. 1996)
\[ k_1 = 2.027 \ h^{-1}; \ k_2 = 1.161 \ h^{-1} \] (water flea Daphnia magna, Wang et al. 1996)

**Half-Lives in the Environment:**

**Air:** \( t_{1/2} = 2.6 \ h \), based on estimated rate constant \( k = 147.2 \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \) at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1991).

**Surface water:** estimated \( t_{1/2} \sim 3.21 \ d \) in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982);
\[ t_{1/2} = 1–4 \ \text{wk} \] in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);
under laboratory conditions in distilled water and river water was completely degraded after 21.3 and 7.3 h, respectively (Mansour et al. 1989; quoted, Montgomery 1993);
\[ t_{1/2} = 3.2 \ d \] to 7–8 months in aquatic environments (Eisler 1985; quoted, Day 1991);
measured rate constant \( k = (24 \pm 4) \ M^{-1} \ s^{-1} \) at pH 4.0, \( k = (13 \pm 1) \ M^{-1} \ s^{-1} \) at pH 4.2, for direct reaction with ozone in water at 26 and 21°C, respectively, with \( t_{1/2} = 1.5 \ h \) at pH 7 (Yao & Haag 1991);
\[ t_{1/2} = 35.6–168 \ h \] in surface water system of a small stream in Iowa by water quality analyses (Kolpin & Kalkhoff 1993);
\[ t_{1/2} = 235 \ d \] at 6°C, \( t_{1/2} = 164 \ d \) at 22°C in darkness, \( t_{1/2} = 59 \ d \) under sunlight conditions for river water at pH 17.3; \( t_{1/2} = 130 \ d \) at 22°C in darkness for filtered river water at pH 7.3 and \( t_{1/2} = 200 \ d \) at 22°C in darkness, \( t_{1/2} = 169 \ d \) under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995)

**Groundwater:** \( t_{1/2} = 6–15 \) months for 0.72–10 \( \mu \)g mL\(^{-1} \) to biodegrade slowly at 25°C (Weidener 1974; quoted, Muir 1991)
reported half-lives or persistence, \( t_{1/2} = 60–150, \ 71, \ 74, \) and 130 d (Bottoni & Funari 1992)

**Sediment:** \( t_{1/2} = 145 \ d \) in a Wisconsin Lake sediment (Armstrong et al. 1967; quoted, Jones et al. 1982; Means et al. 1983) and \( t_{1/2} \sim 30 \ d \) for Chesapeake Bay sediment (Ballantyne et al. 1978; quoted, Jones et al. 1982);
\[ t_{1/2} = 7–28 \ d \] for 0.1 \( \mu \)g mL\(^{-1} \) to rapid degrade in both aerobic and low oxygen systems in estuarine sediment/water at 12–35°C (Jones et al. 1982, quoted, Muir 1991);
\[ t_{1/2} \text{(aerobic)} > 35 \ d \] for 0.1–1.0 \( \mu \)g mL\(^{-1} \) to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)
\[ t_{1/2} = 60–120 \ d \] in surface sediment, \( t_{1/2} = 60–223 \ d \) in subsurface sediment biodegradation \( t_{1/2} = 47–128 \ d \) in the surface and \( t_{1/2} = 70–770 \ d \) in subsurface sediment (Smalling & Aelion 2004)

**Soil:** half-lives in aqueous buffered solutions in soil at 25°C and pH 1, 2, 3, 4, 11, 12, and 13 were reported to be 3.3, 14, 58, 240, 100, 12.5, and 1.5 d, respectively (Armstrong et al. 1967; quoted, Montgomery 1993);
\[ t_{1/2} = 3–5 \ \text{yr} \] in agricultural soils (Armstrong et al. 1967; quoted, Jones et al. 1982);
estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);
\[ t_{1/2} = 1.73, \ 244 \ d \] at 25°C and pH 4 with and without fulvic acid (2%) (Li & Felbeck 1972; quoted, Montgomery 1993);
persistence of 10 months in soil (Morrill et al. 1982);
\[ t_{1/2} = 6.0 \ \text{months} \] at 15°C and \( t_{1/2} = 2.0 \ \text{months} \) at 30°C in soils (Freed & Haque 1973);
persistence of 12 months (Wauchope 1978);
correlated \( t_{1/2} = 37 \ d \) at pH 5.1–7.0, and \( t_{1/2} = 28 \ d \) at pH 7.7–8.2 (Boddington Barn soil, Hance 1979);
\( t_{1/2} = 30 \ d \) at pH 4.6–5.3 and \( t_{1/2} = 40 \ d \) at pH 6.3–8.0 (Triangle soil, Hance 1979);
\[ t_{1/2} = 37 \ d \] in agricultural soils (Dao et al. 1979; quoted, Jones et al. 1982);
estimated first-order \( t_{1/2} = 36.5 \ d \) from biodegradation rate constant \( k = 0.019 \ d^{-1} \) by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
\[ t_{1/2} = 53 \ 113 \ d \] at pH 6.5 at 22°C in a Hatzenbühl soil at pH 4.8 and Neuhofen soil, respectively (Burkhard & Guth 1981; quoted, Montgomery 1993);
\[ t_{1/2} = 1–6 \ \text{months} \] (Jones et al. 1982; quoted, Meakins et al. 1994);
moderately persistent in soils with \( t_{1/2} = 20–100 \ d \) (Willis & McDowell 1982); biodegradation \( t_{1/2} = 71 \ d \) from screening model calculations (Jury et al. 1984; 1987a,b; Jury & Ghodrati 1989);
t½ ~ 6–10 wk (Hartley & Kidd 1987; quoted, Montgomery 1993);
field t½ = 4 wk by using lysimeters (Bowman 1990);
half-lives from soil surfaces: t½ = 655 to > 1000 d in peat soil and t½ = 143–939 d in sandy soil at 20 ± 1°C (Dörfler et al. 1991);
degradation rate constant k = (1.20 ± 0.097) × 10⁻² d⁻¹ with t½ = 57.8 d in control soil and k = (1.01 ± 0.034) × 10⁻² d⁻¹ with t½ = 68.6 d in pretreated soil once only in the laboratory (Walker & Welch 1991); t½ ~ 21 d based on extractable residues in microcosm studies, compared to t½ = 14 d in surface field soil (Winkelmann & Klaine 1991);
selected field t½ = 60 d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);
soil t½ = 130 d (quoted, Pait et al. 1992);
field t½ = 35–50 d in soil and water but may be longer under cold or dry conditions; t½ = 105 to > 200 d under groundwater conditions, depending on test system (Wood et al. 1991; quoted, Tomlin 1994);
reported t½ = 60–150 d, 71 d, 74 d and 130 d (Bottoni & Funari 1992);
first-order k = −0.017 to −0.003 d⁻¹ with corresponding t½ = 41 d in the 0- to 30-cm soil to t½ = 231 d in the 90 to 120-cm soil in Ames, Iowa (Kruger et al. 1993);
dissipation t½ = 71 d from soil surface (Gish et al. 1995); t½ = 105 to > 200 d under groundwater conditions, depending on test system (Wood et al. 1991; quoted, Tomlin 1994);
reported t½ = 60–150 d, 71 d, 74 d and 130 d (Bottoni & Funari 1992);
first-order k = −0.017 to −0.003 d⁻¹ with corresponding t½ = 41 d in the 0- to 30-cm soil to t½ = 231 d in the 90 to 120-cm soil in Ames, Iowa (Kruger et al. 1993);
dissipation t½ = 71 d from soil surface (Gish et al. 1995); t½ = 60 d (Halfon et al. 1996).

**Biota:**
- t½ = 0.03 h in algae,
- t½ = 1.52 d in catfish and
- t½ = 9.5 h in daphnids (Ellgehausen et al. 1980);
- biochemical t½ = 64 d from screening model calculations (Jury et al. 1987b);
- t½ = 25.6 d in bean,
- t½ = 24.3 d in turnips and
- t½ = 14.6 d in oats at 20 ± 1°C from plant surfaces (Dörfler et al. 1991).

### TABLE 17.1.1.4.1

<table>
<thead>
<tr>
<th></th>
<th><strong>Reported vapor pressures of atrazine at various temperatures and the coefficients for the vapor pressure equations</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>log P = A − B/(T/K)</td>
</tr>
<tr>
<td></td>
<td>log P = A − B/(C + T/K)</td>
</tr>
<tr>
<td></td>
<td>log P = A − B/(C + t/°C)</td>
</tr>
<tr>
<td></td>
<td>log P = A − B/(T/K) − C·log (T/K)</td>
</tr>
<tr>
<td>Stammbach 1964</td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>20</td>
<td>4.0 × 10⁻⁵</td>
</tr>
<tr>
<td>extrapolated</td>
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</tr>
<tr>
<td>measured</td>
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</tr>
<tr>
<td>range 50–130°C</td>
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<tr>
<td>Antoine eq.</td>
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<tr>
<td>eq. 1</td>
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</tr>
<tr>
<td>A</td>
<td></td>
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<tr>
<td>B</td>
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<tr>
<td>eq. 1a</td>
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</tr>
<tr>
<td>A</td>
<td></td>
</tr>
<tr>
<td>B</td>
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</tr>
</tbody>
</table>

Knudsen effusion method
FIGURE 17.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for atrazine.
**17.1.1.5 Barban**

![Chemical Structure](image)

Common Name: Barban  
Synonym: Barbamate, Barbane, Carbine, Carbyne, CBN, Chlorinat  
Chemical Name: carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester; 4-chlorobut-2-ynyl 3-chloro-carbanilate; 4-chloro-2-butynyl 3-chlorophenylcarbamate  
Uses: herbicide for post-emergence control of wild oats in wheat, barley, broad beans, field beans, soybeans, peas, sugar beet, flax, lucerne, lentils, mustard, oilseed rape, sunflowers, etc.  
CAS Registry No: 101-27-9  
Molecular Formula: C$_{11}$H$_{9}$Cl$_{2}$NO$_{2}$  
Molecular Weight: 258.101  
Melting Point (°C):  
Boiling Point (°C):  
1.403 (25°C, Hartley & Kidd 1987)  
Molar Volume (cm$^3$/mol):  
262.8 (calculated-Le Bas method at normal boiling point, this work)  
Dissociation Constant pK$_{a}$:  
Enthalpy of Vaporization, $\Delta$H$_v$ (kJ/mol):  
109.1 (Rordorf 1989)  
Enthalpy of Fusion, $\Delta$H$_{fus}$ (kJ/mol):  
26.8 (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: 0.323 (mp at 75°C)  
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):  
15.0 (Swezey & Nex 1961)  
11.0 (20°C, Weber 1972; Worthing & Walker 1987)  
11.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
$1.33 \times 10^{-3}$ (20°C, Weber 1972; Worthing & Walker 1987)  
$5.00 \times 10^{-5}$ (Hartley & Kidd 1987)  
$1.60 \times 10^{-4}$ (Worthing & Walker 1987)  
$5.05 \times 10^{-5}$ (Herbicide Handbook 1989)  
$3.50 \times 10^{-3}$, $1.0 \times 10^{-3}$, 0.019, 0.240, 2.20 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
$\log (P_{v}/Pa) = 14.669 – 5703.8/(T/K)$; measured range 72–150°C (gas saturation-GC, Rordorf 1989)  
Henry’s Law Constant (Pa-m$^3$/mol at 25°C or as indicated):  
$0.00117$ (20°C, calculated-P/C, Muir 1991)  
1.17 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)  
$0.00117$ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, $\log K_{OW}$:
2.68  (selected, Gerstl & Helling 1987)

Bioconcentration Factor, $\log BCF$:
2.20  (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:
3.06  (soil, calculated-S, Kenaga 1980)
2.66  (calculated-MCI $\chi$, Gerstl & Helling 1987)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2} = 6690$ d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: $t_{1/2} = 2.25$ h for 22–99% of 10 $\mu$g/ml to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).
Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987);
persistence of 2 weeks in soil (Edwards 1973; quoted, Morrill et al. 1982);
persistence of about 3 weeks in soil (Herbicide Handbook 1989);
selected field $t_{1/2} = 5$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
17.1.1.6 Benefin

Common Name: Benefin
Synonym: Balan, Bonalan, benfluralin
Chemical Name: \( N\)-butyl-\( N\)-ethyl-\( \alpha,\alpha,\alpha\)-trifluoro-2,6-dinitro-\( p\)-toluidine
Uses: as pre-emergence herbicide for the control of annual grasses and broadleaf weeds in chicory, cucumbers, endive, groundnuts, lettuce, lucerne, and other foliage crops.
CAS Registry No: 1861-40-1
Molecular Formula: \( \text{C}_{13}\text{H}_{16}\text{F}_{3}\text{N}_{3}\text{O}_{4} \)
Molecular Weight: 335.279
Melting Point (°C): 66 (Lide 2003)
Boiling Point (°C): 121–122 (0.5 mmHg), 148–149 at 7 mmHg (Tomlin 1994)
Density (g/cm³ at 20°C): 1.28 (tech., Tomlin 1994)
Molar Volume (cm³/mol): 295.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol): 38.70 (DSC method, Plato & Glasgow 1969)
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 or as indicated):
< 1.0 (Ashton & Crafts 1973)
0.50 (Weber et al. 1980)
1.0 (20°C, selected, Suntio et al. 1988)
0.10 (Herbicide Handbook 1983; Tomlin 1994)
0.10 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.00519 (30°C, Ashton & Crafts 1973)
0.0104 (Herbicide Handbook 1983)
0.0040 (20°C, estimated, Suntio et al. 1988)
0.0087 (Tomlin 1994)
0.0088 (20–25°C, selected, Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.34 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
5.34 (selected, Magee 1991)
5.29 (20°C, pH 7, Tomlin 1994)
5.29 (pH 7, selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
3.36 (calculated-S per Kenaga 1980, this work)
Sorption Partition Coefficient, log $K_{OC}$:

- 4.03 (quoted exptl., Sabljic 1987)
- 4.03, 3.75 (quoted, estimated; Magee 1991)
- 3.95 (soil, Hornsby et al. 1996)
- 2.96 (2.59–3.33) (soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

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

Volatilization:
- Photolysis: atmospheric and aqueous photolysis half-lives were estimated to be 288–864 h (Howard et al. 1991).
- Oxidation: photooxidation $t_\frac{1}{2} \approx 0.782–7.82$ h based on reaction with OH radicals in air (Howard et al. 1991).
- Biodegradation: aerobic $t_\frac{1}{2} \approx 504–2880$ h in soil, and anaerobic soil $t_\frac{1}{2} = 144–480$ h (Howard et al. 1991).

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

Half-Lives in the Environment:

- Air: $t_\frac{1}{2} = 0.782–7.82$ h based on estimated reaction with OH radicals in the gas-phase (Howard et al. 1991).
- Surface water: $t_\frac{1}{2} = 288–864$ h based on observed photolysis by sunlight (Howard et al. 1991).
- Groundwater: $t_\frac{1}{2} = 144–5760$ h based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:
- Soil: $t_\frac{1}{2} = 504–2880$ h based on aerobic solid die-away test data (Howard et al. 1991);
- field $t_\frac{1}{2} = 40$ d (Hornsby et al. 1996).

Biota:
### 17.1.1.7 Bifenox

![Chemical Structure of Bifenox](image)

**Common Name:** Bifenox  
**Synonym:** MC-4379, Modown  
**Chemical Name:** benzoic acid, 5-(2,4-dichlorophenoxy)-2-nitro-, methyl ester; methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate  

**Uses:** selective pre-emergence and post-emergence herbicide to effectively control a wide variety of broadleaf weeds in corn, grain, sorghum, maize, rice, and soybeans.  

**CAS Registry No:** 42576-02-3  
**Molecular Formula:** C<sub>14</sub>H<sub>9</sub>Cl<sub>2</sub>NO<sub>5</sub>  
**Molecular Weight:** 342.131

<table>
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<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>85 (Lide 2003)</td>
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<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>305.5 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>90.5 (Rordorf 1989)</td>
</tr>
<tr>
<td>Dissociation Constant pK&lt;sub&gt;a&lt;/sub&gt;</td>
<td>26.4 (Rordorf 1989)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, ∆H&lt;sub&gt;v&lt;/sub&gt; (kJ/mol)</td>
<td>74.0 (Rordorf 1989)</td>
</tr>
</tbody>
</table>
| Enthalpy of Fusion, ∆H<sub> fus</sub> (kJ/mol) | Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
  | 0.35 (20°C, Weber 1972; Worthing & Walker 1987) |
  | 0.35 (Martin & Worthing 1977; Herbicide Handbook 1978) |
  | 0.35 (Ashton & Crafts 1981; Herbicide Handbook 1989; Budavari 1989) |
  | 0.35 (30°C, Worthing & Walker 1987) |
  | 0.35 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995) |
  | 0.398 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996) |

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Temperature</th>
<th>Reference</th>
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<tbody>
<tr>
<td>0.00032</td>
<td>20°C</td>
<td>Weber 1972; Worthing &amp; Walker 1987</td>
</tr>
<tr>
<td>0.00032</td>
<td>30°C</td>
<td>Ashton &amp; Crafts 1981; Worthing &amp; Hance 1991; Tomlin 1994</td>
</tr>
<tr>
<td>5.40 × 10⁻⁶, 2.0 × 10⁻⁴, 4.40 × 10⁻³, 0.064, 0.67 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)</td>
<td>20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996</td>
<td></td>
</tr>
<tr>
<td>log (P&lt;sub&gt;v&lt;/sub&gt;/Pa) = 14.996 – 6040.4/(T/K); measured range 36.9–85.5°C (solid, gas saturation-GC, Rordorf 1989)</td>
<td>20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996</td>
<td></td>
</tr>
<tr>
<td>log (P&lt;sub&gt;v&lt;/sub&gt;/Pa) = 13.815 – 5582.5/(T/K); measured range 90.5–175°C (liquid, gas saturation-GC, Rordorf 1989)</td>
<td>20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996</td>
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<tr>
<td>0.321</td>
<td>20°C, calculated-P/C, Muir 1991</td>
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<td>0.011</td>
<td>calculated-P/C, Montgomery 1993</td>
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</tr>
<tr>
<td>0.313</td>
<td>calculated-P/C, this work</td>
<td></td>
</tr>
</tbody>
</table>
Herbicides

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 5.63 (selected, Dao et al. 1983)
- 4.50 (Worthing & Hance 1991)
- 4.48 (Montgomery 1993; Tomlin 1994)
- 4.48 (selected, Hansch et al. 1995)
- 5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
- 2.30 (static water, Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 3.05 (calculated-S, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, log $K_{oc}$:
- 3.89 (soil, calculated per Kenaga & Goring, Kenaga 1980)
- 4.0 (estimated-chemical structure, Lohninger 1994)
- 2.70–4.36 (Tomlin 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- Volatilization: estimated $t_{1/2} = 29.8$ d from 1 m depth of water at 30°C (Muir 1991).
- Photolysis: with < 5% degradation by UV light of 290–400 nm in 48 h (Worthing & Hance 1991).
- Oxidation:
  - Hydrolysis: stable in aqueous solution at pH 5.0–7.3 but rapidly hydrolyzed at pH 9.0 both at 22°C (Worthing & Hance 1991).
  - Biodegradation: $t_{1/2} = 2–5$ d for 10 µg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991).
- Biotransformation:
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Soil: $t_{1/2} = 2–5$ d for 10 µg/ml to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991);
  - average $t_{1/2} = 7–14$ d in soils (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);
  - selected field $t_{1/2} = 7.0$ d (Wauchope et al. 1992; Hornsby et al. 1996);
  - average $t_{1/2} = 7–14$ d (Herbicide Handbook 1989);
  - $t_{1/2} = 5–7$ d in soil (Tomlin 1994).
17.1.1.8 Bromacil

Common Name: Bromacil
Synonym: Borea, Bromax, Bromazil, Cynogan, Hyvar, Hyvarex, Krovar I or II, Nalkil, Uragan, Urox B, Uron HX, Weed Blast

Chemical Name: 5-bromo-3-sec-butyl-6-methyluracil; 5-bromo-6-methyl-3-(1-methylpropyl)-2,4-(1H,3H)pyrimidinedione

Uses: Herbicide applied to soil to control annual and perennial grasses, broadleaf weeds, and general vegetation on uncropped land; also used for selective weed control in apple, asparagus, cane fruit, hops, and citrus crops.

CAS Registry No: 314-40-9
Molecular Formula: \( \text{C}_9\text{H}_{13}\text{BrN}_2\text{O}_2 \)
Molecular Weight: 261.115
Melting Point (°C):
- 158 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
- 1.59 (23°C, Tomlin 1994)
- 1.55 (Milne 1995)
Molar Volume (cm\(^3\)/mol):
- 193.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant \( pK_a \):
- 9.10 (Wauchope et al. 1992; Hornsby et al. 1996)
- < 7.0 (Montgomery 1993)
- 9.27 (Tomlin 1994)
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: 0.0496 (mp at 158°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
- 820 (Beste & Humburg 1983; Jury et al. 1983)
- 1064 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984; Gerstl & Helling 1987)
- 626, 775, 1043 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)
- 700, 807, 1287 (at pH 7, 5, 9, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
- 5 × 10\(^{-5}\) (20°C, Weber 1972; Worthing & Walker 1987)
- 3 × 10\(^{-5}\) (estimated, USEPA 1975)
- 0.107 (100°C, Khan 1980)
- 2.9 × 10\(^{-5}\) (Jury et al. 1983)
- 0.00033 (Hartley & Kidd 1987; Worthing & Hance 1991)
- 4 × 10\(^{-5}\) (20–25°C, selected, Wauchope et al. 1992)
- 3.3 × 10\(^{-5}\) (Montgomery 1993)
Herbicides

Henry’s Law Constant (Pa·m³/mol at 25°C at 25°C or as indicated):
- 9.17 × 10⁻⁶ (Beste & Humburg 1983; Jury et al. 1983)
- 0.0019 (20°C, selected, Suntio et al. 1988)
- 1.06 × 10⁻³ (20°C, calculated-P/C, Muir 1991)
- 1.06 × 10⁻³ (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 2.02 (Rao & Davidson 1980)
- 1.33 (selected, Dao et al. 1983)
- 1.84 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
- 1.84, 1.87, 1.90 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)
- 1.85 (selected, Gerstl & Helling 1987)
- 2.11 selected, Magee 1991; Devillers et al. 1996)
- 1.84–2.04 (Montgomery 1993)
- 2.11 (selected, Sangster 1993)
- 1.87, 1.88, 1.63 (at pH 7, 5, 9, Tomlin 1994)
- 2.11 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log $BCF$:
- 0.505 (measured, Kenaga 1980)
- 2.27 (calculated-S, Kenaga 1980)
- 0.477 (calculated-$K_{OC}$, Kenaga 1980)
- 0.51 (Pimephales promelas, Call et al. 1987)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
- 1.86 (soil, Hamaker & Thompson 1972)
- 3.13 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- 1.86 (Rao & Davidson 1980)
- 2.33, 1.34, 1.63 (estimated-S, calculated-S and mp, calculated-$K_{ow}$, Karickhoff 1981)
- 1.61 (sediments average-Freundlich adsorption, Corwin & Farmer 1984)
- 1.41–2.46 (California lake sediments, Corwin & Farmer 1984)
- 1.98, 1.88 (4, 25°C, Semiahmoo soil, in μmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.11, 1.88 (4, 25°C, Adkins soil, in μmol/kg OC, Madhun et al. 1986)
- 1.90, 1.66, 1.75; 1.86, 1.89, 1.34 (estimated-$K_{ow}$; S, Madhum et al. 1986)
- 1.53, 2.73 (quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
- 1.86 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989; Carsel 1989)
- 2.56 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 1.86, 1.80 (reported, estimated as log $K_{OM}$, Magee 1991)
- 1.53, 1.86, 3.13 (soil, quoted values, Bottoni & Funari 1992)
- 1.51 (Montgomery 1993)
- 2.09 (estimated-chemical structure, Lohninger 1994)
- 1.60 (quoted or calculated-QSAR MCI $\chi$, Sabljic et al. 1995)
- 1.43, 1.72 (average values for sediments, soils, Delle Site 2001)
- 1.58, 1.46, 1.53 ( soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 6.3–7.9, average, Delle Site 2001)
- 1.80, 1.72 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, and pH ≤ 7.3 undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2} \sim 10,000$ d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: 115 ppb contaminated water in the presence of TiO₂ and H₂O₂ photodegraded to 6 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).
Oxidation:
Hydrolysis:

Biotransformation:

Biocorcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported $t_{1/2} = 150–158$ and 350 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 7.0$ months at 15°C and $t_{1/2} = 4.5$ months at 30°C in soils (Freed & Haque 1973);

rate constant $k = 0.0038$ d$^{-1}$ with biodegradation $t_{1/2} = 350$ d under field conditions (Rao & Davidson 1980; quoted, Jury et al. 1984);

$t_{1/2} = 350$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} > 100$ d (Willis & McDowell 1982)

$t_{1/2} \approx 5429–46200$ d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

$t_{1/2} = 46200$, 12391, and 5856 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while

$t_{1/2} = 18851$, 9925, and 7588 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat. $t_{1/2} = 5429$, 6789, and 8044 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while $t_{1/2} = 6293$, 5986, and 6784 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhun & Freed 1987) selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 150–180$d and 350 d (Bottoni & Funari 1992).

Biota: biochemical $t_{1/2} = 350$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).
Common Name: Bromoxynil
Synonym: Brittox, Brominal, Brominex, Brommil, Broxynil, Buctril, Chipco crab-kleen, ENT 20852, Nu-lawn weeder, Oxytril M, Partner
Chemical Name: 3,5-dibromo-4-hydroxybenzonitrile; 4-cyano-2,6-dibromophenol
Uses: herbicide for post-emergence control of annual broadleaf weeds and it is often used in combination with other herbicides to extend the spectrum of control.
CAS Registry No: 1689-84-5
Molecular Formula: C$_7$H$_3$Br$_2$NO
Molecular Weight: 276.913
Melting Point (°C):
Boiling Point (°C):
Density (g/cm$^3$ at 20°C):
Molar Volume (cm$^3$/mol):
176.7 (calculated-Le Bas method at normal boiling point, this work)
Dissociation Constant pK$_a$:
4.20 (radiometer/pH meter, Cessna & Grover 1978)
4.06 (Herbicide Handbook 1989; Montgomery 1993)
4.06 (Budavari 1989; Worthing & Hance 1991)
3.86 (Tomlin 1994)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
31.80 (DSC method, Plato 1972)
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: 0.0241 (mp at 190°C)
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
130 (20–25°C, Spencer 1973)
131 (Kenaga 1980)
< 200 (Khan 1980)
130 (20–25°C, Ashton & Crafts 1981)
130 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
130 (Worthing & Walker 1987, Worthing & Hance 1991)
Vapor Pressure (Pa at 25°C or as indicated):
< 0.0010 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.00064 (Herbicide Handbook 1989)
0.00064 (Montgomery 1993)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C or as indicated):
0.14180 (20–25°C, calculated-P/C, Montgomery 1993)
1.36 × 10$^{-3}$ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
2.60 (selected, Dao et al. 1983)
Bioconcentration Factor, log BCF:
1.60 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log KOC:
2.48 (soil, quoted from Kenaga 1980, Bottoni & Funari 1992)
2.48 (calculated, Montgomery 1993)
2.86, 3.06 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k or Half-Lives, t½:
Volatilization:
Photolysis: rate constant of degradation in water, k = 1.04 × 10⁻³ s⁻¹ at pH 8.3 and k = 1.08 × 10⁻³ s⁻¹ at pH 11.6 (Kochany 1992).

Oxidation:
Hydrolysis:

Biodegradation: t½ ~ 24 h for 0.03 µg/mL to biodegrade in runoff water at 20–25°C (Brown et al. 1984; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: t½ ~ 24 h for 0.03 µg mL⁻¹ to biodegrade in runoff water at 20–25°C (Brown et al. 1984; quoted, Muir 1991).

Ground water: reported t½ = 10 d (Bottoni & Funari 1992)

Sediment:

Biota:
17.1.1.10  sec-Bumeton

Common Name: sec-Bumeton
Synonym: etazine, GS14254, secbumeton
Chemical Name: N-ethyl-6-methoxy-\(N'\)-(1-methylpropyl)-1,3,5-triazine-2,4-diamine
CAS Registry No: 26259-45-0
Uses: herbicide
Molecular Formula: C_{10}H_{19}N_{5}O
Molecular Weight: 225.291
Melting Point (°C):
   87  (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
   1.105  (Hartley & Kidd 1987; Worthing & Walker 1987)
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
   4.4  (Worthing 1987)
   4.4, 4.36  (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
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: 0.246 (mp at 87°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   620  (quoted, Kenaga & Goring 1980)
   620  (Ashton & Crafts 1981)
   600  (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
Vapor Pressure (Pa at 25°C or as indicated):
   9.7 \times 10^{-4}  (20°C, Ashton & Crafts 1981; Worthing & Walker 1987)
   9.71 \times 10^{-4}  (20°C, Hartley & Kidd 1987)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
   3.20  (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
   1.20  (fish, Kenaga 1980b)
Sorption Partition Coefficient, log K_{oc}:
   2.54  (soil, calculated, Kenaga & Goring 1980)
   2.11  (soil, calculated, Kenaga 1980b)
   2.18  (soil, pH 7, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
   2.78; 2.29  (soil: quoted, calculated-MCI \(\chi\), Meylan et al. 1992)
   2.78  (soil, calculated-MCI \(\chi\), Sabljic et al. 1995)
2.78; 2.78, 2.55 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Hydrolysis: on hydrolysis at 20°C, $t_{1/2} \sim 30$ d at pH 1, $t_{1/2} = 75$ d at pH 13 (Worthing & Walker 1987).

Half-Lives in the Environment:

Air:
Surface water: on hydrolysis at 20°C, $t_{1/2} \sim 30$ d at pH 1, $t_{1/2} = 75$ d at pH 13 (Worthing & Walker 1987).
Ground water:
Sediment:
Soil: field $t_{1/2} \sim 60$ d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:
17.1.1.11 Butachlor

Common Name: Butachlor
Synonym: Butanex, Butanox, CP 53619, Lambast, Machete, Pillarsete
Chemical Name: N-butoxymethyl-2-chloro-2′,6′-diethylacetanilide; N-(butoxymethyl)-2-chloro-N-(2,6-diethylphenyl)-acetamide
Uses: herbicide for pre-emergence control of most annual grasses, some broadleaf weeds, and many aquatic weeds in both seeded and transplanted rice.
CAS Registry No: 23184-66-9
Molecular Formula: C_{17}H_{26}ClNO_{2}
Molecular Weight: 311.847
Melting Point (°C):
< -5.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
156 (at 0.5 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
387.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
23 (20°C, Weber 1972; Worthing 1987)
20 (Martin & Worthing 1977)
Vapor Pressure (Pa at 25°C or as indicated):
0.0007 (20°C, Weber 1972; Worthing & Walker 1987)
0.0006 (Ashton & Crafts 1981; Herbicide Handbook 1989)
0.0006 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0006 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.00817 (20°C, calculated-P/C, Muir 1991)
0.00814 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₐₜₜ:
4.50 (quoted and recommended, Hansch et al. 1995; quoted, Sabljic et al. 1995)
Bioconcentration Factor, log BCF:
2.06 (calculated-S, Kenaga 1980)
1.03, 0.756 (18, 9 µg/L concn in water; carp, 3–5 d exposure, Wang et al. 1992)
0.38, 0.845 (10, 1 µg/L concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
0.447, 0.845 (10, 1 µg/L concn in water; loach, 3–5 d exposure, Wang et al. 1992)
1.76, 2.02 (2.5, 1.25 µg/L concn in water; grass carp, 3–5 d exposure, Wang et al. 1992)
1.71, 1.90 (5, 2.5 µg/L concn in water; eel, 3–5 d exposure, Wang et al. 1992)
1.99, 2.34 (2.4, 0.4 µg/L concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
0.041, 0.778 (100, 10 µg/L concn in water; freshwater clam, 3–5 d exposure, Wang et al. 1992)

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

- 2.92 (calculated-solubility, Kenaga 1980)
- 2.86 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

- Volatilization: estimated $t_{1/2} \sim 1049$ d from 1 m depth of water at 20°C (Muir 1991).
- Photolysis: $t_{1/2} = 0.8–5.4$ h in distilled water (Chen et al. 1982; quoted, Cessna & Muir 1991).
- Oxidation:
  - Hydrolysis: $t_{1/2} > 2.5$ months for 2 µg/mL to hydrolyze in phosphate buffer at pH 6 and borate buffer at pH 9 both at 25°C (Chen & Chen 1979; quoted, Muir 1991).
- Biodegradation:
- Biotransformation:

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

Half-Lives in the Environment:

- Soil: persists for 6–10 wk in soil (Hartley & Kidd 1987; Tomlin 1994);
  - $t_{1/2} = 4$ to 8 d depending upon soil type (Herbicide Handbook 1989);
  - persists in soil 42–70 d (Worthing & Hance 1991);
  - selected field $t_{1/2} = 12$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
17.1.1.12 Butralin

Common Name: Butralin
Synonym: Amex, Butalin, Rutralin, Sector, Tamex
Chemical Name: N-sec-butyl-4-tert-butyl-2,6-dinitroaniline; 4-(1,1-dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine
Uses: herbicide for pre-emergence control of annual broadleaf weeds and grasses in cotton, beans, barley, rice, soybeans, alliums, vines, ornaments and orchards of fruit and nut trees; also to control suckers on tobacco.
CAS Registry No: 33629-47-9e
Molecular Formula: C_{14}H_{21}N_{3}O_{4}
Molecular Weight: 295.335
Melting Point (°C): 60 (Lide 2003)
Boiling Point (°C): 134–136 (at 0.5 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
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: 0.454 (mp at 60°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{oc}$:
- 3.64 (calculated, Kenaga & Goring 1980; quoted, Kenaga 1980)
- 3.91 (soil, Kenaga & Goring 1980; quoted, Sabljic 1987; Bahnick & Doucette 1988)
- 3.75 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 3.98 (soil, calculated-MCI $s\chi$, Sabljic et al. 1995)
- 3.98; 3.38 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

- **Vaporization:**
  - Photolysis: $t_{1/2} = 8$ h for 25% of 2000 µg/mL to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

- **Oxidation:**
- **Hydrolysis:**
- **Biodegradation:** $t_{1/2} = 24$ d for 0.5 µg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).
- **Biotransformation:**
- **Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**

Half-Lives in the Environment:
- Soil: $t_{1/2} = 24$ d for 0.5 µg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).
17.1.1.13 Butylate

Common Name: Butylate  
Synonym: Butilate, disocarb, Genate, R 1910, Sutan  
Chemical Name: S-ethylbis(diisobutylthiocarbamate; S-ethyl-bis(2-methylpropylcarbamothioate
Uses: herbicide to control annual grass weeds in maize, by pre-plant soil incorporation; also to control some broadleaf weeds.

CAS Registry No: 2008-41-5  
Molecular Formula: C₁₁H₂₃NOS  
Molecular Weight: 217.372  
Melting Point (°C): liquid  
Boiling Point (°C):  
137.5–138 (at 21 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)  
71.0 (at 10 mmHg, Herbicide Handbook 1989)  
Density (g/cm³ at 20°C):  
0.9417 (Milne 1995)  
Molar Volume (cm³/mol):  
280.9 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)  
Dissociation Constant pKₐ:  
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):  
45.0 (Kenaga 1980; Weber et al. 1980)  
46.0 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)  
44.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
36.0 (20°C, Tomlin 1994)  
45.0 (22°C, Milne 1995)  
Vapor Pressure (Pa at 25°C or as indicated):  
1.73 (Ashton & Crafts 1973)  
0.096 (20°C, Hartley & Graham-Bryce 1980)  
0.287 (20°C, GC-RT correlation, Kim 1985)  
0.10 (20°C, selected, Suntio et al. 1988)  
0.17 (Worthing & Hance 1991)  
1.73 (Tomlin 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
0.560 (20°C, calculated-P/C, Suntio et al. 1988)  
Octanol/Water Partition Coefficient, log K₁₀₈:  
4.15 (recommended, Hansch et al. 1995)  
4.17, 4.01, 3.45 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
Bioconcentration Factor, log BCF:
1.86 (calculated-S, Kenaga 1980)
3.06 (calculated-$K_{ow}$ as per Kenaga 1980, this work)

Sorption Partition Coefficient, log $K_{OC}$:
2.73 (soil, Kenaga 1980)
2.73, 4.09 (quoted values, Bottoni & Funari 1992)
2.60 (soil, 20–25°C, selected, Wauchope et al. 1992)
2.11 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
2.39, 2.13 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Half-Lives in the Environment:
Air:
Surface water:
Ground water: reported half-lives or persistence, $t_{1/2} = 11–21$ d (Bottoni & Funari 1992)

Sediment:
Soil: measured dissipation rate k = 3.6 d$^{-1}$ (Nash 1983; quoted, Nash 1988);
estimated dissipation rate k = 23 and 0.61 d$^{-1}$ (Nash 1988);

$\tau_{s} = 1.5–3.0$ wk in several soils under crop growing conditions (Herbicide Handbook 1989);
selected field $\tau_{s} = 13$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
reported $\tau_{s} = 11–21$ d (Bottoni & Funari 1992);
soil $\tau_{s} = 12$ d (quoted, Pait et al. 1992);

$\tau_{s} = 1.5–10$ wk in soil and water (Tomlin 1994);
soil $\tau_{s} = 13$ d (selected, Halfon et al. 1996).

Biota: disappear from the stems and leaves of corn plants 7 to 14 d after application (Herbicide Handbook 1989).


17.1.1.14 Chloramben

![Chemical Structure](attachment:image.png)

Common Name: Chloramben

Synonym: ACP-M-728, Amiben, Amoben, Chlorambed, Chlorambene, M-728, NCI-C00055, Ornamental weeder, Vegaben, Vegiben

Chemical Name: 3-amino-2,5-dichlorobenzoic acid

Uses: pre-emergence or pre-plant herbicide used in many vegetable and field crops to control annual broadleaf weeds and grasses.

CAS Registry No: 133-90-4

Molecular Formula: C₇H₅Cl₂NO₂

Molecular Weight: 206.027

Melting Point (°C):

200 (Lide 2003)

Boiling Point (°C): n/a

Density (g/cm³ at 20°C):

190.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

3.40 (Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_fus (kJ/mol):

38.91 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_fus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.0192 (mp at 200°C)

Water Solubility (g/m³ or mg/L at 25°C):

700 (Spencer 1973; Ashton & Crafts 1981)


700 (Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)


Vapor Pressure (Pa at 25°C or as indicated):

0.933 (100°C, Segal & Sutherland 1967; Spencer 1976)

0.93 (100°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

52.7 (Worthing & Walker 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):

0.274 (calculated-P/C as per Worthing 1987)

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

1.11 (quoted, Rao & Davidson 1980)

1.46 (selected, Dao et al. 1983)

−2.64 (selected, Gerstl & Helling 1987)

1.11 (Magee 1991)

1.11 (Montgomery 1993)

1.11 (Log P database of Hansch & Leo 1987, Sangster 1993)

1.90 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

1.18 (calculated-S, Kenaga 1980)
Sorption Partition Coefficient, log $K_{OC}$:

- $-0.097$ (calculated-$K_{OC}$, Kenaga 1980)

- $1.32$ (soil, Harris & Warren 1964; Farmer 1976)
- $2.08$ (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- $1.78$ (calculated-MCI $\chi$, Gerstl & Helling 1987)
- $1.32$ (reported as log $K_{OM}$, Magee 1991)
- $2.28$ (Montgomery 1993)
- $1.56$ (selected, Lohninger 1994)
- $1.48$ (soil, calculated-MCI $'\chi'$, Sabljic et al. 1995)

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

- Volatilization:

  Photolysis: $t_{1/2} = 6$ h for 206 $\mu$g/mL to degrade in distilled water under sunlight (Sheets 1963; quoted, Cessna & Muir 1991);
  - $t_{1/2} < 2$ d for 16 $\mu$g/mL to degrade in distilled water under sunlight (Hahn et al. 1969; quoted, Cessna & Muir 1991).

- Oxidation:

- Hydrolysis:

- Biodegradation: $t_{1/2} > 70$ d for 50 $\mu$g/mL to degrade in incubated soil with nutrient medium of 3 g/L (Schliebe et al. 1965; quoted, Muir 1991).

- Biotransformation:

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

Half-Lives in the Environment:

- Soil: estimated persistence of 3 months (Kearney et al. 1969; quoted, Jury et al. 1987);
  - $t_{1/2} = 36, 38, 41$, and $20$ d with disappearance rates: $k = 0.0193, 0.0182, 0.0169$ and $0.0347$ d$^{-1}$ at pH 4.3, 5.3, 6.5 and 7.5 (Hamaker 1972; quoted, Nash 1988);
17.1.1.15 Chlorazine

Common Name: Chlorazine
Synonym:
Chemical Name: 6-chloro-\(N,N,N',N'-\)tetraethyl-1,3,5-triazine-2,4-diamine
Uses: herbicide
CAS Registry No: 580-48-3
Molecular Formula: \(C_{11}H_{20}ClN_5\)
Molecular Weight: 257.764
Melting Point (°C):
27 (Howard 1991; Lide 2003)
Boiling Point (°C):
154–156/4.0 mmHg (Howard 1991)
Density (g/cm³):
1.74 (pKₐ of conjugate acid, Howard 1991)
Acid Dissociation Constants, pKₐ:
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: 0.956 (mp at 27°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
3.236 (estimated, Howard 1991)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):
Bioconcentration Factor, log BCF or log \(K_{\text{b}}\):
2.033 (estimated-S, Howard 1991)
Sorption Partition Coefficient, log \(K_{\text{oc}}\):
2.90 (calculated-S, Howard 1991)
Environmental Fate Rate Constants, k, and Half-Lives, \(t_\text{½}\):
Hydrolysis: may be more important at low pH (Howard 1991).
Half-Lives in the Environment:
Air: \(t_\text{½} = 2.5\) h for the vapor phase reaction with OH radicals (estimated, Howard 1991).
17.1.1.16 Chlorbromuron

![Chemical Structure](image)

Common Name: Chlorbromuron
Synonym: Maloran
Chemical Name: 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea
Uses: herbicide
CAS Registry No: 13360-45-7
Molecular Formula: C₉H₁₀BrClN₂O₂
Molecular Weight: 293.544
Melting Point (°C):
- 96 (Lide 2003)
Boiling Point (°C):
Density (g/cm³): 1.69 (Tomlin 1994)
Acid Dissociation Constants, pKₐ:
Molar Volume (cm³/mol):
Enthalpy of Fusion, ∆Hₘᵤₜ (kJ/mol):
Entropy of Fusion, ∆Sₘᵤₜ (J/mol K):
Fugacity Ratio at 25°C, (assuming ∆Sₘᵤₜ = 56 J/mol K) F: 0.201 (mp at 96°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 50 (Kenaga & Goring 1980, Kenaga 1980a; Ashton & Crafts 1981)
- 35; 27.4 (quoted; calculated-MCI χ, Patil 1994)

Vapor Pressure (Pa at 25°C or as indicated):
- 5.33 × 10⁻⁵ (20°C, Ashton & Crafts 1981)
- 5.3 × 10⁻⁵ (Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log Kₜ₉₈:
- 3.06 (quoted, Rao & Davidson 1980)
- 3.09 (shake flask, Brigg 1981)
- 3.09; 3.26 (quoted lit.; calculated-MCI χ, Patil 1994)
- 3.09 (recommended, Hansch et al. 1995)
- 2.86, 2.99, 3.45 (RP-HPLC-RT correlation, CLOGP, HPLC-k’ correlation, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log Kₜₐ:

Bioconcentration Factor, log BCF or log K₆₉:
- 1.83, 1.40 (quoted, calculated, Kenaga 1980b)

Sorption Partition Coefficient, log Kₜ₉₈:
- 2.66 (soil, Kenaga & Goring 1980)
- 2.66, 2.71 (quoted, calculated-K ss, Kenaga 1980b)
- 3.00 (mean value of 5 soils, Rao & Davidson 1980)
- 2.34, 2.94 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
- 2.19–3.61 (range of reported data, Augustijn-Beckers et al. 1994)
Herbicides

2.70 (estimated and recommended, soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.70 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.70, 2.97 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.54, 2.55 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

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

Hydrolysis: slowly hydrolyzed in neutral, slightly acidic, and slightly alkaline media (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: persists in soil > 56 d (Worthing 1983);
\[ t_{1/2} = 45 \text{ d} \] (Hartley & Kidd 1987);
\[ t_{1/2} = 45–120 \text{ d} \] (Tomlin 1994);
\[ t_{1/2} = 21–45 \text{ d} \text{ and } 40 \text{ d} \] (range of reported values and recommended field half-life, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
17.1.1.17 Chlorpropham

Common Name: Chlorpropham
Synonym: Beet-Kleen, Bud-nip, Chlor-IFC, Chloro-IPC, CIPC, Ebanil, ENT 18060, Fasco Wy-hoe, Furloe, Nexoval, Prevenol, Preweed, Sprout-nip, Taterpex
Chemical Name: isopropyl N-(3-chlorophenyl) carbamate; isopropyl 3-chlorocarbanilate
Uses: pre-emergent and post-emergent herbicide used to regulate plant growth and control weeds in carrot, onion, garlic, and other crops.
CAS Registry No: 101-21-3
Molecular Formula: C₁₀H₁₂ClNO₂
Molecular Weight: 213.661
Melting Point (°C): 41 (Lide 2003)
Boiling Point (°C): 149 (at 2 mmHg, Budavari 1989)
Density (g/cm³ at 20°C):
- 1.5388 (Budavari 1989)
Molar Volume (cm³/mol):
- 232.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
- 88.67 (Rordorf 1989)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
- 20.50 (DSC method, Plato & Glasgow 1969)
- 16 (Rordorf 1989)
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.697 (mp at 41°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.470 (Brust 1966)
- 102.3 (shake flask-GC, Freed et al. 1967)
- 108 (20°C, Günther et al. 1968)
- 2.0 (Spencer 1973; quoted, Shiu et al. 1990)
- 0.70 (19°C, shake flask-GC, Bowman & Sans 1979)
- 0.73 (20°C, shake flask-GC, Bowman & Sans 1983a,b)
- 88 (Khan 1980; Ashton & Crafts 1981)
- 80–102 (Weber et al. 1980)
- 89 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 89 (selected, Gerstl & Helling 1987; Montgomery 1993; Lohninger 1994)
- 2.0 (20°C, Worthing & Walker 1987)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.00050 (20°C, Weber 1972; Worthing & Walker 1987)
- 0.00133 (extrapolated, Spencer 1976)
- 0.00133 (Khan 1980)
- 0.00100 (20°C, selected, Suntio et al. 1988)
0.012, 0.30, 5.0, 56, 470 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 16.402 – 5467.7/(T/K); measured range 44.9–140°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 13.753 – 4631.9/(T/K); measured range 44.9–140°C (liquid, gas saturation-GC, Rordorf 1989)
0.00130 (selected, Taylor & Spencer 1990)
0.00107 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00133 (estimated, Montgomery 1993)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
0.0021 (20°C, calculated-P/C, Suntio et al. 1988)
0.0032 (20°C, calculated-P/C, Muir 1991)
0.0021 (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{ow}:
3.06 (Rao & Davidson 1980; Karickhoff 1981)
3.42 (selected, Dao et al. 1983; Gerstl & Helling 1987)
3.51 (shake flask, Mitsutake et al. 1986)
3.10 (selected, Suntio et al. 1988)
3.51 (recommended, Sangster 1993)
3.09 (calculated, Patil 1994)
3.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.70 (calculated-S, Kenaga 1980)
1.52 (calculated-K\text{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.77 (soil, Hamaker & Thompson 1972)
2.57 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.85, 2.80 (estimated-S, Karickhoff 1981)
3.17, 3.08 (estimated-S and mp, Karickhoff 1981)
2.67 (estimated-K_{ow}, Karickhoff 1981)
2.31 (calculated-MCI χ, Gerstl & Helling 1987)
2.32 (calculated-MCI χ and fragment contribution method, Meylan et al. 1992)
2.77, 2.91 (Montgomery 1993)
2.60 (estimated-chemical structure, Lohninger 1994)
2.53 (soil, calculated-MCI 1χ, Sabljic et al. 1995)
2.40, 2.05 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.62 (2.37–2.87) (soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: t½ = 2220 d from 1-m depth of water at 20°C (estimated, Muir 1991).
Oxidation:
Hydrolysis: t½ > 4 months for 4274 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: t½ = 2220 d from 1-m depth of water at 20°C (estimated, Muir 1991).
Photolysis: t½ = 130 h for 4 μg/mL to degrade in distilled water under > 280 nm light (Guzik 1978; quoted, Cessna & Muir 1991)
Direct photolysis t½ = 121 d in distilled water pH 5–7 for a mid-summer day at latitude of 40° (Wolfe et al. 1978)
For 21–76% of 80 μg/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).
Oxidation:
Hydrolysis: t½ > 4 months for 4274 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

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Oxidation:
Hydrolysis: t½ > 4 months for 4274 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

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Biodegradation:

- $t_{1/2} > 1 \text{ wk}$ for $2.10 \mu g/mL$ to hydrolyze in natural waters at $67^\circ \text{C}$ (Schnoor et al. 1982; quoted, Muir 1991).

- Aerobic $t_{1/2} (0.1–5.4 \mu g/mL)$ to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991).

- $k = (3.6–6.7) \times 10^{-10} \text{ mL cell}^{-1} \text{ d}^{-1}$ of different river water samples (Paris et al. 1978; quoted, Scow 1982).

- $t_{1/2} = 120 \text{ d}$ by fungi *Aspergillus fumigatus* and $t_{1/2} = 2.9 \text{ d}$ by bacteria at $28^\circ \text{C}$ (Wolfe et al. 1978).

- $k = 2.5 \times 10^{-4} \text{ L (mg M)}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 120 \text{ d}$ for $2–25 \mu g/mL$ fungus *Aspergillus fumigatus*; $k = 0.1 \text{ L (mg M)}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 2.9 \text{ d}$ for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and $28^\circ \text{C}$ (Wolfe et al. 1978; quoted, Muir 1991).

- $k = (1.6–1.8) \times 10^{-8} \text{ mL cell}^{-1} \text{ d}^{-1}$ of different river water samples (Steen et al. 1979; quoted, Scow 1982).

- $k = (2.6 \pm 0.72) \times 10^{-14} \text{ L cell}^{-1} \text{ h}^{-1}$ in North American waters (Paris et al. 1981; quoted, Battersby 1990).

- $k = (1.3–4.9) \times 10^{-4} \text{ L org}^{-1} \text{ h}^{-1}$ with $t_{1/2} (\text{aerobic}) = 190 \text{ h}$ for $0.1–1.0 \mu g/mL$ to biodegrade in lake water at $22^\circ \text{C}$ (Schnoor et al. 1982; quoted, Muir 1991).

- $t_{1/2} (\text{aerobic}) > 4 \text{ months}$ for $6–7 \mu g/mL$ to biodegrade in river water at $25^\circ \text{C}$ (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:

**Air:**

- Surface water: rate constant $k = 3.6–6.7 \times 10^{-10} \text{ mL cell}^{-1} \text{ d}^{-1}$ from measurements of different river water samples (Paris et al. 1978; quoted, Scow 1982).

- Hydrolysis $t_{1/2} > 1 \times 10^{4} \text{ d}$ based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics.

- Direct photolysis $t_{1/2} = 121 \text{ d}$ assuming a quantum efficiency of 1 and for a mid-summer day at altitude $40^\circ$, and biolysis $t_{1/2} = 120 \text{ d}$ for $1 \text{mg/L}$ of fungus and $t_{1/2} = 2.9 \text{ d}$ for bacteria at $28^\circ \text{C}$ (Wolfe et al. 1978).

- Aerobic $t_{1/2} = 190 \text{ h}$ for $0.1–1.0 \mu g/mL$ to biodegrade in lake water with biodegradation rate of $(1.3–4.9) \times 10^{-2} \text{ L org}^{-1} \text{ h}^{-1}$ at $22^\circ \text{C}$ (Schnoor et al. 1982; quoted, Muir 1991).

- Aerobic $t_{1/2} > 4 \text{ months}$ for $6–7 \mu g \text{ mL}^{-1}$ to biodegrade in river water at $25^\circ \text{C}$ (Stepp et al. 1985; quoted, Muir 1991).

**Ground water:**

- Sediment: aerobic half-life of $10–75 \text{ d}$ for $0.1–5.4 \mu g/mL$ to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991).

- Soil: $t_{1/2} = 65$ and $30 \text{ d}$ soil at $15$ and $29^\circ \text{C}$, respectively (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994).

- Select field $t_{1/2} = 30 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996).

**Biota:**
17.1.1.18 Chlorsulfuron

Common Name: Chlorsulfuron
Synonym: DPX 4189, Finesse, Glean, Telar
Chemical Name: 2-chloro-N-(((4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino)-carbonyl)-benzenesulfonamide; 1-(o-chlorophenyl)-3-(4-methoxy-6-methyl-s-triazin-2-yl)urea
Uses: herbicide to control broadleaf weeds and some grass weeds.
CAS Registry No: 64902-72-3
Molecular Formula: C_{12}H_{12}ClN_{5}O_{4}S
Molecular Weight: 357.773
Melting Point (°C): 176 (Lide 2003)
Density (g/cm³ at 20°C): 
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔHₕ₃ (kJ/mol):
Entropy of Fusion, ΔSₕ₃ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕ₃ = 56 J/mol K), F: 0.0330 (mp at 176°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
300 (at pH 5, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
28000 (at pH 7 with ionic strength 0.05, Herbicide Handbook 1989)
7000 (20–25°C, at pH 7, selected, Hornsby et al. 1996)
60, 7000 (at pH 5, pH 7, Montgomery 1993)
32000 (selected, Armbrust 2000)
Vapor Pressure (Pa at 25°C or as indicated):
6.10 × 10⁻⁴ (Hartley & Kidd 1987)
3.00 × 10⁻⁹ (Worthing & Hance 1991; Tomlin 1994)
1.98 × 10⁻² (20–25°C, Wauchope et al. 1992)
3.11 × 10⁻⁹ (Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
3.60 × 10⁻¹¹ (calculated-P/C, Montgomery 1993)
1.98 × 10⁻⁴ (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
6.79 × 10⁻⁶ (selected, Armbrust 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
−0.84, 0.17, 1.09 (pH 8.4, pH 7.1, pH 4.5, UV, Ribo 1988)
−0.88, 1.05 (pH 8.4, pH 4.5, HPLC, Ribo 1988)
−1.34, 0.74 (pH 7, pH 4.5, Hay 1990)
Bioconcentration Factor, log BCF:
0.622 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log $K_{OC}$:
1.02 (Flanagan silt loam, Montgomery 1993)
1.60 (Tomlin 1994)
2.19 (calculated-MCI $\chi^1$, Sabljic et al. 1995)
1.60 (at pH 7, selected, Hornsby et al. 1996)
1.56 (selected, Armbrust 2000)

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

Vaporization:

Photolysis: assuming first-order kinetics, calculated $t_{1/2} \approx 186$ h for 33 $\mu$g/mL to degrade in distilled water, $t_{1/2} = 31$ h for creek water, $t_{1/2} = 136$ h for silica gel and $t_{1/2} = 115$ h for montmorillonite under sunlight (Herrmann et al. 1985; quoted, Cessna & Muir 1991);
under indoor conditions $t_{1/2} = 92$ h in methanol, $t_{1/2} = 78$ h in distilled water but $t_{1/2} = 18$ h in natural creek water (Herrmann et al. 1985);
reported $t_{1/2} = 18$ h in distilled water at > 290 nm (Montgomery 1993)
aqueous photolysis rate constant, $k = 5.0 \times 10^{-4}$ h$^{-1}$ (Armbrust 2000).

Oxidation:

Hydrolysis: $t_{1/2} = 4–8$ wk at 20°C and pH 5.7–7.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);
stable aqueous hydrolysis rates at pH 7, 9; measured hydroxy radical rate constant for chlorsulfuron $6.9 \times 10^{12}$ M$^{-1}$/h (Armbrust 2000).

Biodegradation: aerobic rate constant, $k = 1.44 \times 10^{-3}$ h$^{-1}$ (Armbrust 2000).

Biotransformation:

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

Half-Lives in the Environment:

Soil: hydrolysis rates will be increased by warm soil temperatures at low pH and in the presence of moisture with an average $t_{1/2} = 4–6$ wk under growing conditions (Hartley & Kidd 1987; Herbicide Handbook 1989) $t_{1/2} = 4–6$ wk for degradation in soil via hydrolysis followed by microbial degradation (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);
degradation rate constants: $k = 0.033$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 21$ d, $k = 0.0315$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 22$ d and for depth 40–60 cm with $t_{1/2} > 150$ d (Soakwaters soil, Walker et al. 1989);
degradation $k = 0.0116$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 60$ d, $k = 0.0120$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 58$ d, and $k = 0.0076$ d$^{-1}$ at depth 40–60 cm with $t_{1/2} = 91$ d (Wharf ground soil, Walker et al. 1989);
degradation $k = 0.0126$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 55$ d, $k = 0.0073$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 95$ d, and $k = 0.0056$ d$^{-1}$ at depth 40–60 cm with $t_{1/2} = 124$ d (Cottage Field soil, Walker et al. 1989);
degradation $k = 0.0147$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 47$ d, $0.0116$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 60$ d, and $k = 0.0047$ d$^{-1}$ at depth 40–60 cm with $t_{1/2} = 147$ d (Hunts Mill soil, Walker et al. 1989);
degradation $0.0094$ d$^{-1}$ (depth 0–20 cm with $t_{1/2} = 74$ d), 0.0096 d$^{-1}$ (depth 20–40 cm with $t_{1/2} = 72$ d) and $0.0082$ d$^{-1}$ (depth 40–60 cm with $t_{1/2} = 85$ d) (Bottom Barn soil, Walker et al. 1989);
degradation $k = 0.0141$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 49$ d, $k = 0.0126$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 55$ d, and $k = 0.0089$ d$^{-1}$ at depth 40–60 cm with $t_{1/2} = 78$ d (Long Ashton soil, Walker et al. 1989);
degradation $k = 0.0144$ d$^{-1}$ at depth 0–20 cm with $t_{1/2} = 48$ d, $k = 0.0126$ d$^{-1}$ at depth 20–40 cm with $t_{1/2} = 55$ d, and $k = 0.0124$ d$^{-1}$ at depth 40–60 cm with $t_{1/2} = 56$ d (Norfolk Agricultural Station soil, Walker et al. 1989)
Herbicides 3509
degradation $k = 0.0248 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 28 \text{ d}$, $k = 0.0289 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 24 \text{ d}$, and $k = 0.0347 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 20 \text{ d}$ (Norfolk Agricultural Station soil, Walker et al. 1989); selected field $t_{1/2} = 40 \text{ d}$ (Hornsby et al. 1996).
17.1.1.19 Chlorotoluron

Common Name: Chlorotoluron
Synonym: C 2242, Clortokem, Deltarol, Dicuran, Highuron, Higaluron, Tolurex
Chemical Name: 3-(3-chloro-\(p\)-tolyl)-1,1-dimethylurea; \(N'\)-(3-chloro-4-methylphenyl)-N,N-dimethylurea
Uses: herbicide to control pre- and post-emergent annual grasses and broadleaf weeds in winter cereals, particularly wheat and barley.
CAS Registry No: 15545-48-9
Molecular Formula: \(C_{10}H_{13}ClN_{2}O\)
Molecular Weight: 212.675
Melting Point (°C):
147 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
1.40 (Tomlin 1994)
Molar Volume (cm\(^3\)/mol):
192 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994)
Dissociation Constant \(p_K_a\):
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: 0.0635 (mp at 147°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
10.0 (20°C, Spencer 1973)
70.0 (Martin & Worthing 1977)
10.0 (20°C, Khan 1980)
70.0 (20°C, Ashton & Crafts 1981)
56.4, 80.6, 99.1 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
70.0 (20°C, Hartley & Kidd 1987; Worthing & Walker 1991)
90.0 (Spurlock 1992; Spurlock & Biggar 1994)
10660 (calculated, Patil 1994)
74.0 (Tomlin 1994)
49.3 (predicted-AQUAFAC, Lee et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
4.8 \times 10^{-6} (20°C, Khan 1980)
1.7 \times 10^{-5} (20°C, Ashton & Crafts 1981)
1.7 \times 10^{-5} (20°C, Hartley & Kidd 1987)
1.7 \times 10^{-5} (Tomlin 1994; selected, Halfon et al. 1996)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
5.17 \times 10^{-5} (20°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
2.41 (shake flask-UV, Briggs 1981)
2.54 (Dao et al. 1983; Spurlock 1992; Spurlock & Biggar 1994)
2.33, 2.34, 2.32 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
2.41 (shake flask, Mitsutake et al. 1986)
2.0 (shake flask, pH 7, Baker et al. 1992)
Herbicides

2.241 (calculated, Evelyne et al. 1992)
2.41 (recommended, Sangster 1993)
2.25 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
0.26 (calculated, Patil 1994)
2.50 (Tomlin 1994)
2.41 (recommended, Hansch et al. 1995)
2.38, 2.44 (shake flask-UV, calculated-RP-HPLC-k’ correlation, Liu & Qian 1995)
2.25, 2.49, 2.42 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
2.0 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.75 (calculated-S, Kenaga 1980)
2.09, 2.16 (cuticle/water 24 h: tomato, pepper, Chaumat et al. 1991)
2.01, 2.15 (cuticle/water 24 h: box tree, pear, Chaumat et al. 1991)
1.30, 2.09 (cuticle/water 24 h: vanilla, Chaumat et al. 1991)
2.09, 2.16 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K OC:
2.62 (soil, calculated-S, Kenaga 1980)
1.78 (reported as log K OM, Briggs 1981)
2.75, 2.62 (4°C, 25°C, Semiahmoo soil, in µmol/kg OC, batch equilibrium-sorption isotherm-liquid scintillation spectrometer LSS, Madhun et al. 1986)
2.57, 2.43 (4°C, 25°C, Adkins soil, in µmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
2.48, 2.18; 2.54, 2.50 (estimated-K OW; solubility, Madhun et al. 1986)
2.81, 2.58 (exptl., calculated-K OW Liu & Qian 1995)
2.02 (soil, calculated-MCI 1\chi, Sabljic et al. 1995)
2.02; 2.05, 2.15 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.00, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
2.14, 2.36 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: calculated t½ > 200 d at pH 5, 7, 9 and 30°C (Tomlin 1994).
Biodegradation: Biological degradation rate followed a first order kinetics with t½ = 21.6 d by raw water microflora from River Nile, t½ = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)
Biotransformation: 4% of the selected 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted 50% of chlorotoluron (100 mg/L) in 5-d experiment. (Vroumsia et al. 1996)
Bioconcentration, Uptake (k 1) and Elimination (k 2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: Biological degradation t½ = 21.6 d by raw water microflora from River Nile, t½ = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)
Ground water:
Sediment:
Soil: t½ = 4 wk in the moist silty loam at (25 ± 1)°C (Smith & Briggs 1978); t½ ~ 200–4000 d in loamy sand and peat for 25–35°C as follows (Madhun & Freed 1987):
t½ = 4340, 904, and 381 d at 25, 30, and 35°C, respectively; at herbicide concn at 5 µg/kg, while t½ = 1335, 524, and 266 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat, t½ = 2306, 1245, and 618 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while t½ = 1949, 1024, and 582 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahmoo mucky peat (Madhun & Freed 1987)
degradation by microorganism in biometer systems, \( t_{\text{d}} = 93 \) d in silty sand standard metabolism experiments, 
\( t_{\text{d}} = 140 \) d corrected standard conditions, \( t_{\text{d}} = 110 \) d in simulated outdoor conditions; \( t_{\text{d}} = 40 \) d in silty loam standard conditions, \( t_{\text{d}} = 60 \) d corrected standard conditions, \( t_{\text{d}} = 31 \) d in simulated outdoor conditions; at constant soil moisture and \( 20^\circ \text{C} \). Degradation by microorganism in small lysimeter systems: 
\( t_{\text{d}} = 52 \) d outdoor fallow, \( t_{\text{d}} = 14 \) d outdoor barley in silty sand, and \( t_{\text{d}} = 49 \) d outdoor fallow, \( t_{\text{d}} = 38 \) d outdoor barley in silty loam (Rüdel et al. 1993)

\( t_{\text{d}} = 30–40 \) d in soil (Tomlin 1994);

\( t_{\text{d}} = 135 \) d (selected, Halfon et al. 1996).

Biota:
17.1.1.20 Cyanazine

**Common Name:** Cyanazine
**Synonym:** Bladex, 90DF, DW 3418, Fortrok, Fortrol, Payze, SD 15418, WL 19805

**Chemical Name:** 2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methyl-propionitrile

**Uses:** herbicide to control annual grasses and broadleaf weeds in cereals, cotton, maize, onions, peanuts, peas, potatoes, soybeans, sugar cane, and wheat fallow.

**CAS Registry No:** 21725-46-2

**Molecular Formula:** C$_9$H$_{13}$ClN$_6$

**Molecular Weight:** 240.692

**Melting Point (°C):**

168°C (Lide 2003)

**Boiling Point (°C):**

**Density (g/cm$^3$ at 20°C):**

**Molar Volume (cm$^3$/mol):**

**Dissociation Constant:**

- 1.00 (pK$_a$, Weber et al. 1980; Willis & McDowell 1982)
- 12.9 (pK$_a$, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.63, 1.1 (pK$_a$, Montgomery 1993)

**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: 0.0395 (mp at 168°C)**

**Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):**

- 150 (selected, Schnoor & McAvoy 1981; Schnoor 1992)
- 171 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
- 171 (Budavari 1989; Milne 1995)
- 6046 (calculated, Patil 1994)
- 45 (calculated-group contribution fragmentation method, Kühne et al. 1995)

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

- $5.33 \times 10^{-7}$ (selected, Schnoor & McAvoy 1981; Schnoor 1992)
- $1.00 \times 10^{-5}$ (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)
- $\ln (P/\text{Pa}) = 25.7–10913/(T/K)$, temp range 65.7–92°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)
- $5.21 \times 10^{-6}$ (Worthing & Walker 1987)
- $2.13 \times 10^{-7}$ (20°C, Budavari 1989)
- $2.13 \times 10^{-7}$ (20°C, Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
- $2.87 \times 10^{-7}$ (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- $3.00 \times 10^{-7}$ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 2.18 (Kenaga & Goring 1980)
- 1.80, 1.66 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.22 (selected, Magee 1991)
- 1.80, 2.24 (Montgomery 1993)
- 2.22 (recommended, Sangster 1993)
- 0.79 (calculated, Patil 1994)
- 2.10 (Tomlin 1994)
- 2.22 (recommended, Hansch et al. 1995)
- 2.04 (shake flask-UV, Liu & Qian 1995)
- 1.64, 1.29, 3.02 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
- 1.70 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
- 1.53 (calculated-S, Kenaga 1980)
- 1.00 (calculated-$K_{OC}$, Kenaga 1980)
- 1.48 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

Sorption Partition Coefficient, log $K_{OC}$:
- 2.30 (Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981; Sabljic 1987; Bahnick & Doucette 1988)
- 2.41 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (Georgia’s Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.71, 1.75, 1.85 (estimated-S, calculated-S and mp, calculated-$K_{OW}$, Karickhoff 1981)
- 0.48–1.48 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 2.57, 2.26 (soil, quoted, Madhun et al. 1986)
- 2.36, 2.09; 2.33, 1.75 (estimated-reported $K_{OW}$; estimated-reported solubilities, Madhun et al. 1986)
- 2.23 (soil, screening model calculations, Jury et al. 1987b)
- 2.35 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 2.30, 2.16 (reported, estimated as log $K_{OC}$, Magee 1991)
- 2.23, 2.26, 2.30 (soil, quoted values, Bottoni & Funari 1992)
- 1.58–2.63 (Montgomery 1993)
- 2.54 (selected, Lohninger 1994)
- 2.05, 2.11 (exptl., calculated-$K_{OW}$, Liu & Qian 1995)
- 2.28 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.28; 2.33, 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.14, 2.19 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 5.6–8.0, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation:
- Biodegradation: aerobic $t_{1/2} = 14$ d for 0.06 $\mu$g/mL to degrade in pond water and $t_{1/2} > 28$ d in pond sediment both at 10–20°C (Roberts 1974; quoted, Muir 1991).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Half-Lives in the Environment:

Air:
Surface water: aerobic $t_{1/2} = 14$ d for 0.06 µg/mL to degrade in pond water at 10–20°C (Roberts 1974; quoted, Muir 1991).

Ground water: reported half-lives or persistence, $t_{1/2} = 10–29, 14$ and 108 d (Bottoni & Funari 1992)

Sediment: aerobic $t_{1/2} > 28$ d for 0.06 µg/mL to slowly degrade in pond sediment at 10–20°C (Roberts 1974; quoted, Muir 1991).

Soil: $t_{1/2} = 2$ wk in soil (Beynon et al. 1972; quoted, Tomlin 1994);
persistence of 12 months in soil (Wauchope 1978);
$t_{1/2} = 13.5$ d from screening model calculations (Jury et al. 1987b);
$t_{1/2} = 12–15$ d in sandy loam soils and $t_{1/2} = 20–25$ d in silt and clay loam soils (Herbicide Handbook 1989; quoted, Montgomery 1993);
disappearance $t_{1/2} = 181$ d from the upper 15 cm on a clay loam Ontario soil in 1987 and $t_{1/2} = 90$ d in 1988 with $t_{1/2}(\text{calc}) = 27$ and 12 d, respectively (Frank et al. 1991);
reported $t_{1/2} = 10–29$ d, 13 d and 108 d (Bottoni & Funari 1992);
selected field $t_{1/2} = 14$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
soil $t_{1/2} = 19$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2} = 13.5$ d from screening model calculations (Jury et al. 1987b).

<table>
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<th>$t/°C$</th>
<th>$P/Pa$</th>
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<td>77.5</td>
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<td>85.8</td>
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<td>92.0</td>
<td>0.0181</td>
</tr>
<tr>
<td>20</td>
<td>$1. \times 10^{-5}$</td>
</tr>
</tbody>
</table>

$\ln P = A - B/(T/K)$
FIGURE 17.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for cyanazine.
17.1.1.21 2,4-D

(See also Chapter 13, Carboxylic Acids)

Common Name: 2,4-D
Synonym: 2,4-Dichlorophenoxyacetic acid
Chemical Name: 2,4-dichlorophenoxyacetic acid
Uses: post-emergence control of annual and perennial broadleaf weeds in cereals, maize, sorghum, grassland, established turf, grass seed crops, orchards, cranberries, asparagus, sugar cane, rice, forestry, and on noncropland, etc.

CAS Registry No: 94-75-7
Molecular Formula: C₈H₆Cl₂O₃, Cl₂C₆H₃OCH₂COOH
Molecular Weight: 221.038

Melting Point (°C):
140.5 (Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Lide 2003)

Boiling Point (°C):
160 (at 0.4 mmHg, Dean 1985)
215 (Neely & Blau 1985)

Density (g/cm³ at 25°C):
1.416 (Montgomery 1993)

Molar Volume (cm³/mol):
209.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₘ:
2.73 (potentiometric method, Nelson & Faust 1969)
2.87 (spectrophotometric method, Cessna & Grover 1978)
2.80 (Reinert & Rogers 1984; selected, Wauchope et al. 1992)
2.64 (Dean 1985; Haag & Yao 1992; Lee et al. 1993)
2.61–3.31 (Howard 1991)
2.97 (Sangster 1993)
3.10 (Kollig 1993)
2.64–3.31 (Montgomery 1993)

Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
93.89 (Rordorf 1989)

Enthalpy of Fusion ∆Hᶠus (kJ/mol):
38.074 (DSC method, Plato & Glasgow 1969)
39.6 (Rordorf 1989)

Entropy of Fusion, ∆Sᶠus (J/mol K):

Fugacity Ratio at 25°C (assuming ∆Sᶠus = 56 J/mol K), F: 0.0736 (mp at 140.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
890 (Hodgman 1952; Hamaker 1975; Verschueren 1983; Montgomery 1993)
522 (shake flask-UV, Leopold et al. 1960)
725 (Bailey & White et al. 1965)
725, 400, 900, 550 (Gunther et al. 1968)
900 (Herbicide Handbook 1974; Wauchope 1978; Kenaga 1980a,b; Kenaga & Goring 1980)
600 (20°C, Khan 1980)
620–900 (Weber et al. 1980)
470 (20–25°C, pH 5.6, Geyer et al. 1981)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

\[
\begin{align*}
8.0 \times 10^{-5} & \quad \text{(Hamaker 1975)} \\
0.180 & \text{–} 1.69 & \quad \text{(transpiration method, Spencer 1976)} \\
53.0 & \quad \text{(160°C, Hartley & Kidd 1983, 1987)} \\
8.0 \times 10^{-5} & \quad \text{(recommended, Neely & Blau 1985; Lyman 1985)} \\
1.0 & \quad \text{(20°C, selected, Suntio et al. 1988)} \\
6.0 \times 10^{-6} & \quad \text{(selected, Nash 1989)} \\
4.10 \times 10^{-3}, 2.0 \times 10^{-3}, 0.058, 1.10, 13.0 & \quad \text{(25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)} \\
\log (P/P_0) = 17.56 - 6544.1/(T/K); & \quad \text{measured range 70.2–135°C (solid, gas saturation-GC, Rordorf 1989)} \\
\log (P/P_0) = 13.558 - 4904.6/(T/K); & \quad \text{measured range 140–196°C (liquid, gas saturation-GC, Rordorf 1989)} \\
0.20, 0.0032 & \quad \text{(quoted, estimated from Henry’s law constant, Howard 1991)} \\
5.6 \times 10^{-5} & \quad \text{(selected, Mackay & Stiver 1991)} \\
1.40, 3.2 \times 10^{-3} & \quad \text{(quoted, estimated from HLC, Howard 1991)} \\
1.33 \times 10^{-3}, 8.0 \times 10^{-3}, 1.07 \times 10^{-3}, 1.07 \times 10^{-3} & \quad \text{(20–25°C, quoted lit; selected, Wauchope et al. 1992)} \\
0.627 & \quad \text{(Montgomery 1993)} \\
0.011 & \quad \text{(Tomlin 1994)} \\
\end{align*}
\]

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated):

\[
\begin{align*}
1.36 \times 10^{-3} & \quad \text{(calculated-P/C, Jury et al. 1983)} \\
1.39 \times 10^{-5} & \quad \text{(calculated-P/C, Jury et al. 1987a, Jury & Ghodrati 1989)} \\
0.55 & \quad \text{(20°C, calculated-P/C, Suntio et al. 1988)} \\
0.0015 & \quad \text{(calculated, Nash 1989)} \\
1.03 \times 10^{-3} & \quad \text{(calculated-bond contribution, Howard 1991)} \\
6.80, 0.853 & \quad \text{(pH 1, pH 7 at 20°C, wetted wall column-GC, Rice et al. 1997b)} \\
1.82 \times 10^{-7} & \quad \text{(quoted lit., Armbrust 2000)} \\
\end{align*}
\]

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

\[
\begin{align*}
2.81 & \quad \text{(shake flask-UV, Fujita et al. 1964)} \\
2.59 & \quad \text{(electrometric titration, Freese et al. 1979)} \\
1.57 & \quad \text{(Kenaga & Goring 1980; Kenaga 1980b)} \\
2.74 & \quad \text{(selected, Dao et al. 1983)} \\
2.81 & \quad \text{(20°C, Verschueren 1983)} \\
1.57, 4.88 & \quad \text{(shake flask-OECD 1981 Guidelines, Geyer et al. 1984)} \\
2.65 & \quad \text{(shake flask, log P Database, Hansch & Leo 1987)} \\
2.50 & \quad \text{(OECD 1981 method, Kerler & Schönherr 1988)} \\
2.649 & \quad \text{(liquid/liquid-countercurrent-chromatography, Ichmann et al. 1993)} \\
2.81 & \quad \text{(recommended, Sangster 1993)} \\
1.44–4.18 & \quad \text{(quoted lit. range, Montgomery 1993)} \\
2.58–2.83 & \quad \text{(pH 1, Tomlin 1994)} \\
2.81 & \quad \text{(selected, Hansch et al. 1995)} \\
0.59 & \quad \text{(RP-HPLC-RT correlation, CLOGP, Calculated-S, Finizio et al. 1997)} \\
\end{align*}
\]
Herbicides

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 1.11, –0.097 (calculated-S, $K_{OW}$, Kenaga 1980a)
- 2.46, 1.30 (beef fat, fish, Kenaga 1980b)
- 0.778, 1.94 (algae Chlorella: expl. 24 h exposure, calculated-S, Geyer et al. 1981)
- 0.778 (algae, Freitag et al. 1982)
- < 1.00 (golden orfe, Freitag et al. 1982)
- 1.23 (activated sludge, Freitag et al. 1982)
- 0.0 (fish, microcosm conditions, Garten & Trabalka 1983;)
- 0.778, 1.23 (algae, calculated-$K_{OW}$, Geyer et al. 1984)
- 1.23 (algae, Geyer et al. 1984)
- 1.11 (calculated, Isensee 1991)
- –5.00 (bluegill sunfish and channel catfish, Howard 1991)
- –2.70 (frog tadpoles, Howard 1991)
- –3.0, –2.52 (pH 7.8, seaweeds, Howard 1991)
- 0.778, 0.85 (quoted: alga, fish, Howard 1991)
- 0.0, 0.505 (catfish Ictalurus melas, water flea Daphnia magna, wet wt basis, Wang et al. 1996)

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

- 1.51 (Hamaker 1975)
- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
- 1.30, 2.11 (quoted, Kenaga & Goring 1980)
- 1.30 (quoted, Kenaga 1980b)
- 1.76 (quoted, average value of 3 soils, McCall et al. 1980)
- 2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
- 1.29 (soil, Neely & Blau 1985)
- 1.30 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.61 (soil, quoted, Sabljic 1987)
- 1.75, 2.00 (quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
- 2.59 (HPLC-k' correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
- 1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oeppen et al. 1991)
- 1.30–1.78, 1.30–2.0, 1.72 (soil, quoted lit. values, Bottoni & Funari 1992)
- 1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted values, Wauchope et al. 1992)
- 1.30 (soil, selected, Wauchope et al. 1992)
- 0.68 (calculated-$K_{OW}$, Kollig 1993)
- 1.68–2.73 (Montgomery 1993)
- 1.66 (calculated-QSAR MCI $\chi$, Sabljic et al. 1995)
- 2.09, 1.04, 1.40, 0.778 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.65, 1.36, 1.37, 0.899 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 1.652 (second generation Eurosoil ES-1, HPLC-k' correlation, Gawlik et al. 2000)
- 1.68 (soil, quoted, Armbrust 2000)
- 1.79, 1.77 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH 2.8–8.0, average, Delle Site 2001)
- 2.16, 2.13 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH 2.8–5.0, average, Delle Site 2001)
- 1.68, 1.68 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH $> 5.0$, average, Delle Site 2001)

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

Volatilization: volatilization from water is negligible, calculated volatilization $t_{1/2} = 660$ d (from 1 cm) and $t_{1/2} = 7.1$ yr (from 10 cm) from soil (Howard 1991).
Photolysis: aqueous photolysis $t_{1/2} = 2–4$ d when irradiated at 356 nm, $t_{1/2} = 50$ min in water when irradiated at 254 nm and $t_{1/2} = 29–43$ d when exposed to September sunlight (Howard 1991); aqueous photolysis rate constant, $k = 2.2 \times 10^{-1}$ h$^{-1}$ (Armbrust 2000).

Oxidation:
photooxidation $t_{1/2} = 1.8–18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$$k({\text{aq.}}) = (1.0–2.3) \times 10^{-3} \text{ M}^{-1} \text{s}^{-1}$$

for direct reaction with ozone in water at pH 1.5–2.9 and 21 ± 1°C, with $t_{1/2} = 3.9$ h at pH 7 (Yao & Haag 1991);

$$k({\text{calc}}) = 5.0 \times 10^3 \text{ M}^{-1} \text{s}^{-1}$$

(Howard & Yao 1992)

$$k_{{\text{OH}}(\text{aq.})} = (1.6–10) \times 10^{-5} \text{ M}^{-1} \text{s}^{-1}$$

for reaction with hydroxyl radical in irradiated field water both in the laboratory and sunlight rice paddies (Mabury & Crosby 1996; quoted, Armbrust 2000);

$$k_{{\text{OH}}(\text{aq.})} = 8.4 \times 10^{-13} \text{ M}^{-1} \text{h}^{-1}$$

at pH 5, 7, 9; measured hydroxyl radical rate constant for 2,4-D, (Armbrust 2000)

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at pH > 8 (Howard 1991).

Biodegradation:

$$k = 0.7–14.0 \text{ d}^{-1}$$

and $t_{1/2} = 10$ to > 50 d in clear to murky river water with lag time ranges from 6–12 d (Nesbitt & Watson 1980a);

$$t_{1/2} = 4$$ d in river with nutrient and suspended sediments and $t_{1/2} = 10$ d with a lag time of 5 d for filtered river water (Nesbitt & Watson 1980b);

degradation kinetics not first-order, time for 50% decomposition in six soils: Commerce 5 d, Catlin 1.5 d, Keith 3.9 d, Cecil 3.0 d, Walla-Walla 2.5 d and Fargo 8.5 d, with an average time of 4 d (McCall et al. 1981)

aerobic degradation $k = 0.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 97.0$ d for control system, $k = 9.5 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 3.1$ d for metabolism, $k = 16.2 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 1.8$ d for co-metabolism; anaerobic degradation $k = 0.24 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 120$ d for control system, $k = 0.21 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 135$ d for metabolism, $k = 0.42 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 69$ d for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

$$k = (3.6–28.8) \times 10^{-6} \text{ mL cell}^{-1} \text{d}^{-1}$$


$$k < 0.14–0.07 \text{ d}^{-1}$$

in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985)

$$k = (0.058 \pm 0.006) \text{ d}^{-1}$$

in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985)

$$k = 0.08–0.46 \text{ d}^{-1}$$

in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$$t_{1/2} (\text{aq. aerobic}) = 240–1200$$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980; selected, Howard et al. 1991);

$$t_{1/2} (\text{anaerobic}) = 672–4320$$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

$$k = 0.035 \text{ d}^{-1}$$

in die-away test, $k = 0.029 \text{ d}^{-1}$ in CO$_2$ evolution test, in soil and $k = 6.9 \times 10^{-1} \text{ mL (g bacteria)}^{-1} \text{d}^{-1}$

by activated sludge cultures (Scow 1982);

$$t_{1/2} = 18$$ to over 50 d in clear river water, and $t_{1/2} = 10$ to 25 d in muddy river water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to half-lives of 1.8–3.1 d under aerobic conditions and 69–135 d under anaerobic conditions (Howard 1991)

$$k(\text{aerobic}) = 5.25 \times 10^{-3} \text{ h}^{-1}$$

(Armbrust 2000).

Biotransformation:

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

$$k_1 = 0.0092 \text{ h}^{-1}$$

; $k_2 = 0.0092 \text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

$$k_1 = 0.8560 \text{ h}^{-1}$$

; $k_2 = 0.2690 \text{ h}^{-1}$ (Water flea *Daphnia magna*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8–18$ h, based on estimated rate constant for the reaction with OH radical (Howard et al. 1991); photooxidation $t_{1/2} = 23.9$ h for reactions with OH radical in air (Howard 1991).

Surface water: $t_{1/2} = 48–96$ h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Baur & Bovey 1974; selected, Howard et al. 1991); degradation $t_{1/2} = 14$ d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of 1 µg mL$^{-1}$ in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

$$t_{1/2} = 1.8$$ and 3.1 d for cometabolism and metabolism, respectively, easily degraded under aerobic conditions; $t_{1/2} = 69$ and 135 d under anaerobic conditions (Liu et al. 1981).
Herbicides

Typical biodegradation $t_{1/2} = 10$ to $< 50$ d with longer expected in oligotrophic waters, photolysis $t_{1/2} = 29$–43 d for water solutions irradiated at sunlight (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} = 6$ to 170 d (Muir 1991);
rate constant $k_{(exptl)} = (1.0$–$2.3) \times 10^7$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 1.5–2.9 and 21°C,
with $t_{1/2} = 3.9$ h at pH 7 (Yao & Haag 1991);
rate constant $k_{(calc)} = 5 \times 10^9$ M$^{-1}$ s$^{-1}$ for the reaction with hydroxyl radical in aqueous solution (Haag & Yao 1992);
$t_{1/2} = 2$–4 d when irradiated at $\lambda = 356$ nm in aqueous solution (Montgomery 1993).

Ground water: $t_{1/2} = 480$–4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)
reported $t_{1/2} = 4, 15, 1$–35, 7–21 d (Bottoni & Funari 1992)
Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} = 6$ to 170 d (Muir 1991).
Soil: degradation $t_{1/2} = 5.0$ and 4.0 d in Quachita Highlands' forest and grassland soil respectively, $t_{1/2} = 4$ d in Gross Timbers Forest soil, average $t_{1/2} = 4$ d in 3 soils (shake flask, Altim & Stritzke 1973);
field $t_{1/2} = 5.2$ d in Arid range (Lane et al. 1977; quoted, Nash 1983);
field $t_{1/2} = 19$ d in Dykland soil (Stewart & Gaul 1977; quoted, Nash 1983);
lab. $t_{1/2} = 5.5$ d in Naff soil (Wilson & Cheng 1978; quoted, Nash 1983);
non-persistent in soil with $t_{1/2} < 20$ d (Willis & McDowell 1982);
field $t_{1/2} = 15$ d in soil (Jury et al. 1983, 1987a,b; Jury & Ghodrati 1989);
persistence of one month in soil (Jury et al. 1987);
$t_{1/2} = 240$–1200 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
biodegradation $t_{1/2} < 1$ d to several weeks, $t_{1/2} = 3.9$ and 11.5 d in 2 moist soils and $t_{1/2} = 9.4$ to 254 d in the same soils under dry conditions (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} = 6$ to 170 d (Muir 1991);
reported $t_{1/2} = 4, 15, 1$–35 and 7–21 d (Bottoni & Funari 1992);
field $t_{1/2} = 2$–16 d, with a selected value of 10 d (Wauchope et al. 1992);
soil $t_{1/2} = 18$ d (Pait et al. 1992);
rate constants for Amsterdam silt loam at soil depth 0–30 cm: $k = 0.0053$ d$^{-1}$ at 10°C, $k = 0.0046$ d$^{-1}$ at 17°C and $k = 0.0127$ d$^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 7, 7$, and 2 d; at soil depth 30–60 cm: $k = 0.00012$ d$^{-1}$ at 10°C, $k = 0.0044$ d$^{-1}$ at 17°C and $k = 0.0077$ d$^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 273, 8$, and 4 d; and at soil depth 60–120 cm: $k = 0.00005$ d$^{-1}$ at 10°C, $k = 0.0013$ d$^{-1}$ at 17°C and $k = 0.0022$ d$^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 593, 25$, and 12 d (Veeh et al. 1996).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).
17.1.1.22 Dalapon

Common Name: Dalapon
Synonym: Alatex, Basinex P, Crisapon, D-Granulat, Dawson-Rae, Ded-Weed, Dowpon, DPA, Gramevin, Kenapon, Liropon, Proprop, Radapon
Chemical Name: 2,2-dichloropropanoic acid; 2,2-dichloropropionic acid; α-dichloropropanoic acid; α,α-dichloropropionic acid
Uses: selective systemic herbicide to control perennial and annual grasses on noncropland, fruits, vegetables, and some aquatic weeds.
CAS Registry No: 75-99-0
Molecular Formula: C₃H₄Cl₂O₂
Molecular Weight: 143.2969
Melting Point (°C): liquid
Boiling Point (°C):
- 98–99 (sodium salt at 20 mmHg, Budavari 1989)
Density (g/cm³ at 20°C):
- 1.389 (Nelson & Faust 1969; quoted, Kenaga 1974; Montgomery 1993)
- 1.4014 (Budavari 1989; Milne 1995)
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
- 1.84 (potentiometric titration, Nelson & Faust 1969; Freed 1976; Hornsby et al. 1996)
- 1.74 (Kenaga 1974; quoted, Howard 1991)
- 1.74–1.84 (Worthing & Hance 1991; Tomlin 1994)
- 2.06 (Yao & Haag 1991; Haag & Yao 1992)
- 1.84 (free acid, Montgomery 1993)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 900,000 (Woodford & Evans 1963; Bailey & White 1965)
- > 800,000 (Kenaga 1974)
- 502,000 (Martin & Worthing 1977)
- 450,000 (Weber et al. 1980; Budavari 1989)
- 501,200 (Garten & Trabalka 1983)
- 431,850 (selected, Gerstl & Helling 1987)
- 500,000 (Reinert 1989)
- 450,000–900,000 (Montgomery 1993)
- 900,000 (20–25°C, selected, Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
- 16.0 (calculated from high temp., Foy 1976)
- 1.0 × 10⁻³ (Worthing & Hance 1991; Tomlin 1994)
- 0.0 (20–25°C, selected, Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 6.50 × 10⁻³ (Hine & Mookerjee 1975)
- 0.608 (calculated, Montgomery 1993)
4.56 × 10\(^{-3}\) (calculated-P/C as per Howard 1991, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log \(K_{OW}\):

- 0.76 (Kenaga 1974)
- 0.78 (Kenaga 1980)
- 1.34 (selected, Dao et al. 1983)
- –2.76 (selected, Gerstl & Helling 1987)
- 1.48 (Reinert 1989)
- 0.78 (selected, Hansch et al. 1995)
- 1.47 (LOGSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{OA}\):

Bioconcentration Factor, log BCF:

- 0.477 (dalapon sodium salt in fish, Kenaga 1974)
- –0.444 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 0.301 (estimated-\(K_{OW}\), Lyman et al. 1982; quoted, Howard 1991)

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

- 0.477 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 0.97 (calculated-MCI \(\chi\), Gerstl & Helling 1987)
- 2.13 (Reinert 1989)
- 0.48, 2.13 (soil, quoted values, Bottoni & Funari 1992)
- 0.27–2.18 (calculated, Montgomery 1993)
- 0.40 (soil, calculated-MCI \(1\chi\), Sabljic et al. 1995)
- 0.0 (soil, 20–25°C, selected, Hornsby et al. 1996)

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

Volatilization:

Photolysis:

Oxidation:

- photooxidation \(t_{\frac{1}{2}} = 289–2893\) h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- \(k(aq.) = 4.6 \times 10^8\) M\(^{-1}\) s\(^{-1}\) for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
- \(k(aq.) \leq 0.005\) M\(^{-1}\) s\(^{-1}\) for direct reaction with ozone in water at pH 6.4 and 22°C, with a half-life of > 2 yr at pH 7 (Yao & Haag 1991).
- \(k(aq.) = (7.3 \pm 0.3) \times 10^7\) M\(^{-1}\) s\(^{-1}\) for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic \(t_{\frac{1}{2}} = 336–1440\) h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991); rate constant \(k = 0.047\) d\(^{-1}\) by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982); aqueous anaerobic \(t_{\frac{1}{2}} = 1344–5760\) 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: \(t_{\frac{1}{2}} = 289–2893\) 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: \(t_{\frac{1}{2}} = 336–1440\) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
measured rate constant $k \leq 0.0005 \text{ M}^{-1} \text{s}^{-1}$ for direct reaction with ozone in water at pH 6.4 and 22°C, with a $t_{1/2} \geq 2 \text{ yr}$ at pH 7 (Yao & Haag 1991).

Groundwater: $t_{1/2} = 672–2880$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

reported $t_{1/2} = 30$ d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 7–8$ d in soil (Kaufman 1966; quoted, Kaufman 1976);

persistence across 43 soils from < 2 wk to > 8 wk (Day et al. 1963; quoted, Kaufman 1976);

$t_{1/2} = 336–1440$ h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

estimated persistence of 8 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 wk in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 2 wk in growing season in most agricultural soils (Herbicide Handbook 1974; quoted, Kaufman 1976);

estimated first-order $t_{1/2} = 15$ d from biodegradation rate constant $k = 0.047 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

non-persistent in soil with $t_{1/2} < 20$ d (Willis & McDowell 1982);

reported half-life or persistence, 30 d (Verschuren 1983; Bottoni & Funari 1992);

field $t_{1/2} = 30$ d at 20–25°C (selected, Hornsby et al. 1996).

Biota:
Common Name: 2,4-DB
Synonym: Butoxon, Butyrac, Butyrac 118, Embutox, Legumex D
Chemical Name: 4-(2,4-dichlorophenoxy)butanoic acid; 4-(2,4-dichlorophenoxy)butyric acid
Uses: herbicide for post-emergence control of many annual and perennial broadleaf weeds in lucerne, clovers, undersown cereals, grassland, forage legumes, soybeans, and groundnuts.
CAS Registry No: 94-82-6
Molecular Formula: C_{10}H_{10}Cl_{2}O_{3}
Molecular Weight: 249.090
Melting Point (°C): 118 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol): 254.2 (calculate-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
5.95 (Bailey & White 1965; Que Hee et al. 1981)
4.80 (Worthing & Walker 1987; Hornsby et al. 1996)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
91.29 (Rordorf 1989)
Enthalpy of Fusion, ΔHₕᵤ (kJ/mol):
33.6 (Rordorf 1989)
Entropy of Fusion, ΔSₕᵤ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕᵤ = 56 J/mol K), F: 0.122 (mp at 118°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
82.3 (Bailey & White 1965)
53 (rm. temp., Melnikov 1971)
46 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
46 (Weber et al. 1980)
46 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)
46 (20–25°C, selected, Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
negligible (Hartley & Kidd 1987)
1.0 × 10⁻⁵, 5.90 × 10⁻⁴, 0.019, 0.38, 5.20 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 17.692 – 6760.5/(T/K); measured range 80–120°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 12.682 – 4768.7/(T/K); measured range 125–196°C (liquid, gas saturation-GC, Rordorf 1989)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₒₜₖ:
3.53 (shake flask-HPLC/UV, Jafvert et al. 1990)
3.53 (selected, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF:
1.85 (calculated-S, Kenaga 1980)
2.21 (calculated-log Kₒₜₖ as per Mackay 1982, this work)

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

- 2.72 (soil, calculated-S, Kenaga 1980)
- 1.3 (organic carbon, Wauchope et al. 1991)
- 2.64 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:

- **Volatileization:**
  - Oxidation: photolysis $t_{1/2} = 6–60$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
  - Biodegradation: aqueous aerobic $t_{1/2} = 24–168$ h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96–672$ 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:** $t_{1/2} = 6–60$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; Howard et al. 1991).
- **Surface water:** $t_{1/2} = 24–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- **Groundwater:** $t_{1/2} = 48–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  - Reported $t_{1/2} < 7$ d (Bottoni & Funari 1992)
- **Sediment:**
  - Soil: $t_{1/2} = 24–168$ h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991)
  - Selected $t_{1/2} = 10$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
  - $t_{1/2} < 7$ d (Worthing & Hance 1991; Bottoni & Funari 1992);
  - Field $t_{1/2} = 5$ d (20–25°C, selected, Hornsby et al. 1996).

- **Biota:**
### 17.1.1.24 Diallate

**Common Name:** Diallate  
*Synonym:* Avadex, CP 15336, DATC, Pyradex  
**Chemical Name:** S-(2,3-dichloroallyl)diisopropyl(thiocarbamate); S-(2,3-dichloro-2-propenyl)bis(1-methylethyl)-carbamothioate

**Uses:** pre-emergent and selective herbicide to control wild oats and blackgrass in barley, corn, flax, lentils, peas, potatoes, soybeans, and sugar beets.

**CAS Registry No:** 2303-16-4  
**Molecular Formula:** C_{10}H_{17}Cl_{2}N_{2}O_{S}  
**Molecular Weight:** 270.219

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<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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<tr>
<td>Melting Point (°C)</td>
<td>25–30 (Herbicide Handbook 1989; Montgomery 1993)</td>
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<tr>
<td>Boiling Point (°C)</td>
<td>97 (at 0.15 mmHg, Herbicide Handbook 1989)</td>
<td>108 (at 0.25 mmHg, Herbicide Handbook 1989; Montgomery 1993)</td>
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<tr>
<td></td>
<td>150 (at 9 mmHg, Howard 1991; Milne 1995; Montgomery 1993)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>1.188 (25°C, Hartley &amp; Kidd 1987; Montgomery 1993)</td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>305.1 (calculated-Le Bas method at normal boiling point)</td>
<td></td>
</tr>
<tr>
<td>Dissociation Constant pKₐ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔHₘᵤₜ (kJ/mol)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ΔSₘᵤ (J/mol K)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ΔSₘᵤ = 56 J/mol K), F</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40.0 (Günther et al. 1968)</td>
<td></td>
<td>14.0 (Ashton &amp; Crafts 1973, 1981)</td>
</tr>
<tr>
<td>40.0 (rm. temp., Spencer 1973; Khan 1980)</td>
<td></td>
<td>40.0 (Martin &amp; Worthing 1977; Hartley &amp; Kidd 1987; Montgomery 1993; Milne 1995)</td>
</tr>
<tr>
<td>40.5 (20–25°C, shake flask-GC, Kanazawa 1981)</td>
<td></td>
<td>52.5 (Garten &amp; Trabalka 1983)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C or as indicated):</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.020 (Ashton &amp; Crafts 1973; Herbicide Handbook 1989)</td>
<td></td>
<td>0.0337 (20°C, GC-RT correlation, Kim 1985)</td>
</tr>
<tr>
<td>0.0117 (20°C, Hartley &amp; Graham-Bryce 1980)</td>
<td></td>
<td>0.020 (Hartley &amp; Kidd 1987)</td>
</tr>
<tr>
<td>0.013 (20°C, selected, Suntio et al. 1988)</td>
<td></td>
<td>0.020 (20°C, Montgomery 1993)</td>
</tr>
<tr>
<td>0.020 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.250 (20°C, calculated-P/C, Suntio et al. 1988)</td>
<td></td>
<td>0.385 (calculated-P/C, Howard 1991)</td>
</tr>
<tr>
<td>0.253 (20–25°C, calculated-P/C, Montgomery 1993)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 5.23 (estimated, USEPA 1988; quoted, Howard 1991)
- 3.29 (calculated, Montgomery 1993)
- 3.67 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:
- 2.08 (calculated-K$_{OC}$, Kenaga 1980)

Sorption Partition Coefficient, log $K_{OC}$:
- 3.28 (soil, Grover 1974)
- 2.96, 2.46, 2.59, 2.49, 2.65 (Melfort loam, Weyburn sandy loam, Regina clay, Indian Head sandy loam, Asquith loamy sand, Grover et al. 1979)
- 3.28 (soil, measured value, Kenaga 1980; Kenaga & Goring 1980)
- 3.00 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.77 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
- 2.28 (Montgomery 1993)
- 3.52 (selected, Lohninger 1994)
- 3.28 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 3.28, 3.21, 2.66 (soil, cis-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 3.28; 3.21, 2.65 (soil, trans-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:
- Photolysis: $t_{1/2} = 4$ h, < 1% of 135 µg/mL to degrade in distilled water under > 300 nm light (Ruzo & Casida 1985; quoted, Cessna & Muir 1991).
- Oxidation: photooxidation $t_{1/2} = 0.58–5.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
- Hydrolysis: neutral hydrolysis rate constant $k = (1.2 \pm 0.7) \times 10^{-5}$ h$^{-1}$ with a calculated first-order $t_{1/2} = 6.6$ yr at pH 7 (Ellington et al. 1987, 1988);
  - first-order $t_{1/2} = 6.6$ yr, based on measured first-order base catalyzed hydrolysis rate constant at pH 7 (Ellington et al. 1987; quoted, Howard et al. 1991)
  - $t_{1/2} = 2400$ d at pH 2, $t_{1/2} = 2500$ d at pH 7 and $t_{1/2} = 32$ d at pH 12 in natural waters (Capel & Larson 1995).
- Biodegradation: aqueous aerobic $t_{1/2} = 252–2160$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1008–8640$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)
  - $t_{1/2}$(aerobic) = 11 d, $t_{1/2}$(anaerobic) = 42 d in natural waters (Capel & Larson 1995)

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

Half-Lives in the Environment:
- Air: $t_{1/2} = 0.58–5.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
- Surface water: $t_{1/2} = 252–2160$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)
  - Biodegradation $t_{1/2}$(aerobic) = 11 d, $t_{1/2}$(anaerobic) = 42 d, hydrolysis $t_{1/2} = 2400$ d at pH 2, $t_{1/2} = 2500$ d at pH 7 and $t_{1/2} = 32$ d at pH 12 in natural waters (Capel & Larson 1995)

Sediment:
Soil: $t_{1/2} = 252–2160$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991; Montgomery 1993);
$\quad t_{1/2} = 30$ d (Hartley & Kidd 1987; quoted, Montgomery 1993);
$\quad$ selected field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:
17.1.1.25 Dicamba

Common Name: Dicamba

Synonym: Banex, Banvel, Banvel D, Brush buster, Dianat, MDBA, Mediben

Chemical Name: 3,6-dichloro-2-methoxybenzoic acid; 3,6-dichloro- o-anisic acid

Uses: systemic pre-emergent and post-emergent herbicide to control both annual and perennial broadleaf weeds.

CAS Registry No: 1918-00-9

Molecular Formula: C₈H₆Cl₂O₃

Molecular Weight: 221.038

Melting Point (°C):
115 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
207.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:
1.94 (Kearney & Kaufman 1975; Spencer 1982; Lee et al. 1993)
1.95 (Worthing & Hance 1991; Montgomery 1993; Caux et al. 1993)
1.87 (Tomlin 1994)
1.91 (Hornsby et al. 1996)

Enthalpy of Vaporization, ∆HV (kJ/mol):
77.85 (Rordorf 1989)

Enthalpy of Fusion, ∆H_fus (kJ/mol):
22.59 (DSC method, Plato & Glasgow 1969)
19.1 (Rordorf 1989)

Entropy of Fusion, ∆S_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F: 0.131 (mp at 115°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
7900 (Freed 1966; Verschueren 1983)
5600 (20°C, selected, Suntio et al. 1988)
4410, 221 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)
8310 (selected., Armbrust 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00454 (Ashton & Crafts 1973; 1981)
0.00267 (Baur & Bovey 1974; Spencer 1976)
0.49 (20°C, Hartley & Graham-Bryce 1980; Khan 1980)
< 0.00013 (20–25°C, Weber et al. 1980; Willis & McDowell 1982)
0.00453 (Herbicide Handbook 1983, 1989; Worthing & Hance 1991)
0.0045 (Hartley & Kidd 1987; Tomlin 1994)
0.50 (100°C, Budavari 1989)
2.90 × 10⁻³, 6.40 × 10⁻², 0.88, 8.60, 63.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/\text{Pa}) = 14.706 - 5139.1/(T/K); measured range 60.1–110°C (solid, gas saturation-GC, Rordorf 1989)
log (P/\text{Pa}) = 11.911 - 4067.0/(T/K); measured range 115–176°C (liquid, gas saturation-GC, Rordorf 1989)
0.50 \quad (20°C, selected, Taylor & Spencer 1990)
0.0045 \quad (20°C, Montgomery 1993)

Henry’s Law Constant (\text{Pa-m}^3/\text{mol at 25°C or as indicated}):  
0.00012 \quad (20°C, calculated-P/C, Suntio et al. 1988)  
0.0248 \quad (calculated-P/C, Taylor & Glotfelty 1988)  
0.0918 \quad (Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)  
2.2 \times 10^{-5} \quad (calculated-P/C, Nash 1989)  
1.22 \times 10^{-4} \quad (20–25°C, calculated-P/C, Montgomery 1993)  
0.00012, 0.000154 \quad (20, 25°C, quoted, Caux et al. 1993)  
4.46 \times 10^{-5} \quad (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log \text{K}_{\text{OW}}:  
0.477 \quad (Rao & Davidson 1980)  
2.41 \quad (selected, Dao et al. 1983)  
2.21 \quad (shake flask, Log P Database, Hansch & Leo 1985, 1987)  
–1.69 \quad (selected, Gerstl & Helling 1987)  
3.01 \quad (selected, Travis & Arms 1988)  
2.46 \quad (Reinert 1989)  
2.49 \quad (shake flask-HPLC/UV, Jafvert et al. 1990)  
2.46 \quad (EPA Environmental Fate one-liner database Version 3.04, Lee et al. 1993)  
2.21 \quad (recommended, Sangster 1993)  
0.48 \quad (Montgomery 1993)  
–0.80 \quad (pH 7, Tomlin 1994)  
2.21 \quad (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:  
0.699 \quad (calculated-S, Kenaga 1980)  
–2.00 \quad (calculated-\text{K}_{\text{OC}}, Kenaga 1980)  
–4.58 \quad (beef biotransfer factor logB_b, correlated-\text{K}_{\text{OW}}, Oehler & Ivie 1980)  
–4.60 \quad (milk biotransfer factor logB_m, correlated-\text{K}_{\text{OW}}, Oehler & Ivie 1980)  
1.450 \quad (estimated-\text{K}_{\text{OW}} per Hansch & Leo 1985, Lyman et al. 1982)  
0.903 \quad (estimated-S per Suntio et al. 1988, Lyman et al. 1982)

Sorption Partition Coefficient, log \text{K}_{\text{OC}}:  
–0.398 \quad (soil, quoted exptl., Kenaga 1980)  
1.63 \quad (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
0.342 \quad (av. soils/sediments, Rao & Davidson 1980)  
–0.40, 2.08 \quad (quoted, calculated-MCI χ, Gerstl & Helling 1987)  
0.34 \quad (soil, screening model calculations, Jury et al. 1987b)  
2.67 \quad (\text{K}_{\text{OC}} = 470 reported, Reinert 1989)  
0.643 \quad (soil, estimated, Shirmohammadi et al. 1989)  
–1.00 \quad (selected, USDA 1989; quoted, Neary et al. 1993)  
0.30 \quad (organic carbon, Wauchope et al. 1991)  
–0.40, 1.62, 0.18, 0.34 \quad (soil, quoted values, Bottoni & Funari 1992)  
1.50; 1.46 \quad (soil, quoted exptl.; calculated-MCI χ and fragment contribution Meylan et al. 1992)  
–0.40, 0.34 \quad (Montgomery 1993)  
0.30 \quad (Tomlin 1994)  
1.50 \quad (quoted or calculated-QSAR MCI χ, Sabljic et al. 1995)  
1.114 \quad (quoted lit., Armbrust 2000)

Sorption Partition Coefficient, log \text{K}_{\text{OM}}:  
2.74 \quad (organo-clay DODMA140-SA, sorption isotherm, Zhao et al. 1996)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatileization:
Photolysis: aqueous photolysis rate constant $k = 7.5 \times 10^{-4}$ h$^{-1}$ (Armbrust 2000).

Oxidation: photooxidation $t_{1/2} = 2.4$–6.0 d, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991);
measured hydroxy radical reaction rate constant for dicamba $4.8 \times 10^{12}$ M$^{-1}$/h (Armbrust 2000).

Hydrolysis: $t_{1/2} > 133$ d for 2 µg mL$^{-1}$ to hydrolyze in dark sterile pond water at 37–39°C (Scifres et al. 1973; quoted, Muir 1991);
stable aqueous hydrolysis rates at pH 5, 7, 9 (Armbrust 2000).

Biodegradation: $t_{1/2} = 60$ d to $>160$ d for 100 µg mL$^{-1}$ to degrade in pond sediment/water under lighted conditions at 20–30°C (Scifres et al. 1973; quoted, Muir 1991); under lab. conditions using nonsterile sandy loam, silty clay, or heavy clay soil, 50% of applied dicamba degraded within 2 weeks; however in sterilized (via heating) soil, over 90% of applied dicamba was recovered after 4 weeks, suggesting that microbes were responsible for the decomposition (Smith 1973; quoted, Howard 1991);
$t_{1/2} > 25$ d for 5.85 mg of labeled dicamba to plants to degrade following washoff from plants and sands in model ecosystem (derived from data of Yu et al. 1975; Muir 1991);
first-order $k = 0.022$ d$^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
rate of biodegradation in soil generally increases with temperature and soil moisture (up to 50%) and tends to be faster when the soil is slightly acidic (Herbicide Handbook 1983; quoted, Howard 1991);
aerobic rate constant $k = 1.60 \times 10^{-3}$ h$^{-1}$ (Armbrust 2000).

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

Half-Lives in the Environment:
Air: $t_{1/2} \sim 2.42$ d for reaction with hydroxyl radicals (estimated, Eisenreich et al. 1981; quoted, Caux et al. 1993)
$t_{1/2} = 2.42$–6.0 d, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:
Ground water: $t_{1/2} = 23.5$ d determined under batch conditions at 28°C, $t_{1/2} = 38$ d at 20°C, and $t_{1/2} = 151$ d at 12°C and were all higher than $t_{1/2} \sim 13.5$ d from the decrease in column effluent concentrations over time (Comfort et al. 1992);
reported $t_{1/2} = 14$–433, 201 and 25 d (Bottoni & Funari 1992)
$t_{1/2} < 7$ d in surface water (Caux et al. 1993).

Sediment:
Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987a);
$t_{1/2} = 59, 19,$ and 17 d with disappearance rates: $k = 0.0117, 0.036$ and 0.041 d$^{-1}$ at pH 4.3, 5.3 and 6.5 (Hamaker 1972; quoted, Nash 1988);
persistence of 2 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
degradation $t_{1/2} = 32$ d and 17 d in Quachita Highlands = forest and grassland soil respectively, $t_{1/2} = 26$ d in Gross Timbers Forest soil, average $t_{1/2} = 25$ d in 3 soils (Altom & Stritzke 1973);
first-order $t_{1/2} \sim 31.5$ d in soil from biodegradation rate constant $k = 0.022$ d$^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
nonpersistent in soils with $t_{1/2} < 20$ d (Willis & McDowell 1982);
mean $t_{1/2} = 14$ d under lab. conditions from review of persistence literature, while the mean $t_{1/2} = 8$ d under field conditions (Rao & Davidson 1982; quoted, Howard 1991);
non-persistent with $t_{1/2} < 20$ d in soil (Willis & McDowell 1982);
$t_{1/2} = 14$ d from screening model calculations (Jury et al. 1987b);
non-persistent with $t_{1/2} < 20$ d in soil (Willis & McDowell 1982);
$t_{1/2} < 14$ d under conditions amenable to rapid metabolism (Herbicide Handbook 1989);
selected $t_{1/2} = 14$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
$t_{1/2} < 14$–25 d (Worthing & Hance 1991; quoted, Montgomery 1993);
Herbicides

reported $t_{1/2} = 20$ d, $25$ d and $14$–$433$ d (Bottoni & Funari 1992);
$t_{1/2} = 4$–$555$ d with a mean $t_{1/2} = 24$ d (Caux et al. 1993);
$t_{1/2} < 14$ d (Tomlin 1994).

Biota: biochemical $t_{1/2} = 14$ d from screening model calculations (Jury et al. 1987b);
average $t_{1/2} = 25$ d in the forest (USDA 1989; quoted, Neary et al. 1993);
biological $t_{1/2} = 0.64$ h (Caux et al. 1993).
17.1.1.26 Dichlobenil

Common Name: Dichlobenil

Synonym: Barrier 2G, Barrier 50W, Casoron, DBN, DCB, Decabane, Du-Sprex, Dyclomec, NIA 5996, Niagara 5006, Niagara 5996, Norosac

Chemical Name: 2,6-dichlorobenzonitrile

Uses: soil applied herbicide to control many annual and perennial broadleaf weeds.

CAS Registry No: 1194-65-6

Molecular Formula: C₇H₃Cl₂N

Molecular Weight: 172.012

Melting Point (°C): 144.5 (Lide 2003)


Density (g/cm³ at 20°C): > 1.0 (Milne 1995)

Molar Volume (cm³/mol): 148.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, ΔHV (kJ/mol): 65.74 (Rordorf 1989)

Enthalpy of Fusion, ΔHfus (kJ/mol):

25.94 (DSC method, Plato & Glasgow 1969)
34.33 (Verloop 1972)
24.2 (Rordorf 1989)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.0672 (mp at 144.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

18 (20°C, Günther et al. 1968; Weber 1972; Verloop 1972; Spencer 1982; Verschueren 1983)
25 (Günther et al. 1968; Montgomery 1993)
18 (Martin & Worthing 1977; Herbicide Handbook 1978)
18 (Wauchope 1978; Khan 1980; Burkhard & Guth 1981)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.072 (20°C, effusion manometer technique, Barnsley & Rosher 1961)
0.0667 (20°C, Weber 1972; Worthing & Walker 1987)
0.0004 (20°C, Spencer 1976)
0.0066 (20°C, effusion method, Spencer 1976)
0.0733 (20–25°C, Weber et al. 1980)
0.073 (20°C, Hartley & Kidd 1987)
0.070 (20°C, selected, Suntio et al. 1988)
0.110, 1.80, 20.0, 160, 970 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (Pₚ/Pa) = 14.787 – 4698.2/(T/K); measured range 32.4–125°C (solid, gas saturation-GC, Rordorf 1989)
log (P_t/P_a) = 11.754 – 3434.1/(T/K); measured range 32.4–125°C (liquid, gas saturation-GC, Rordorf 1989)

0.133 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0733 (Montgomery 1993)

0.088 (20°C, gas saturation, Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

0.700 (20°C, volatilization rate, Burkhard & Guth 1981)

0.669 (20°C, calculated-P/C, Suntio et al. 1988)

0.637 (20°C, calculated-P/C, Muir 1991)

0.669 (20–25°C, calculated-P/C, Montgomery 1993)

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

2.90 (Rao & Davidson 1980; selected, Suntio et al. 1988, Magee 1991)

2.57; 2.65 (RP-HPLC-RT correlation; shake flask, Eadsforth & Moser 1983)

3.06 (shake flask, Geyer et al. 1984)

2.94 (Hansch & Leo 1985)

1.63 (Reinert 1989)

2.98 (selected, Dao et al. 1983, Gerstl & Helling 1987)

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

2.90 (recommended, Sangster 1993)

2.70 (Tomlin 1994)

2.74 (recommended, Hansch et al. 1995)

2.95 (RP-HPLC-RT correlation, Nakamura et al. 2001)

2.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.74 (fish in static water, Kenaga 1975; Kenaga & Goring 1980)

2.08 (calculated-S, Kenaga 1980; quoted, Isensee 1991)

1.08 (calculated-K_{OC}, Kenaga 1980)

1.18–1.60 (fish, Freitag et al. 1982)

1.30 (algae, Freitag et al. 1982)

1.72 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)

2.03–2.32 (Montgomery 1993)

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

2.91 (potting soil with 22% organic content, Massini 1961)

2.08 (sandy loam with 5% organic content, Massini 1961)

2.37 (soil, Hamaker & Thompson 1972–1987)

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

2.35 (Rao & Davidson 1980)

2.94 (soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)

2.37, 1.45 (quoted, calculated-MCI χ, Gerstl & Helling 1987)

2.96 (Reinert 1989)

2.37; 2.31 (reported as log K_{OM}; estimated as log K_{OM}, Magee 1991)

2.21, 2.57–2.96 (soil, quoted values, Bottoni & Funari 1992)


2.60 (estimated-chemical structure, Lohninger 1994)

2.31 (soil, calculated-MCI χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatileization: t_{1/2} ~ 7.4 d, based on Henry’s law constant for a model river 1-m deep with a wind velocity of 3 m/s and flowing at 1 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991);

2.03–2.32 (Montgomery 1993)

Photolysis: photolytic t_{1/2} = 15 d in water (Tomlin 1994).
Oxidation: photooxidation $t_{1/2} = 92$ d in air, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Hydrolysis:

Biodegradation: $t_{1/2} \sim 7$ d for 5 $\mu$g/mL to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 92$ d, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water:

Ground water: reported $t_{1/2} = 44–360$ d (Bottoni & Funari 1992)

Sediment: $t_{1/2} \sim 7$ d for 5 $\mu$g/mL to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Soil: estimated persistence of 4 months (Kearney et al. 1969; quoted, Jury et al. 1987);

- $t_{1/2} = 1–6$ months in soil depending on soil type (Beynon & Wright 1972; Verloop 1972; quoted, Tomlin 1994);
- persistence of 4 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
- persistence of 4 months (Wauchope 1978);
- $t_{1/2} = 1.5$ to 12 months depending upon soil type (Herbicide Handbook 1989);

selected $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

reported $t_{1/2} = 45–360$ d (Bottoni & Funari 1992).

Biota:
**17.1.1.27 Dichlorprop**

Common Name: Dichlorprop  
Synonym: Cornox RK, dichlorprop, Dikofag DP, 2,4-DP, Hedonal DP, Polymone  
Chemical Name: (±)-2-(2,4-dichlorophenoxy)propanoic acid; (±)-2-(2,4-dichlorophenoxy)propionic acid  
Uses: herbicide and growth regulator to control annual broadleaf and grass weeds; also to control aquatic weeds and chemical maintenance of embankments and roadside verges.  
CAS Registry No: 120-36-5  
Molecular Formula: C₉H₈Cl₂O₃  
Molecular Weight: 235.064  
Melting Point (°C):  
117.5 (Lide 2003)  
Boiling Point (°C):  
1.64 (25°C, Bailey & White 1965)  
1.42 (Herbicide Handbook 1989; Tomlin 1994)  
Density (g/cm³ at 20°C):  
Dissociation Constant pKₐ:  
2.855 (Cessna & Grover 1978)  
2.86 (Wauchope et al. 1992; Hornsby et al. 1996)  
3.00 (Tomlin 1994)  
Enthalpy of Vaporization, ΔHV (kJ/mol):  
127.9 (Rordorf 1989)  
Enthalpy of Fusion, ΔHfus (kJ/mol):  
34.31 (DSC method, Plato 1972)  
30.9 (Rordorf 1989)  
Entropy of Fusion, ΔSfus (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.124 (mp at 117.5°C)  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
350 (20°C, Woodford & Evans 1963; Spencer 1973)  
350 (Martin & Worthing 1977)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
4.50 × 10⁻⁴ (20°C, Hartley & Kidd 1987)  
2.90 × 10⁻⁷, 4.10 × 10⁻⁵, 2.8 × 10⁻³, 0.11, 2.80 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
\[ \log (P/Pa) = 21.26 - 8289.2/(T/K); \text{measured range 95.7–118°C (solid, gas saturation-GC, Rordorf 1989)} \]  
\[ \log (P/Pa) = 17.14 - 6682.8/(T/K); \text{measured range 120–150°C (liquid, gas saturation-GC, Rordorf 1989)} \]  
< 1.0 × 10⁻⁵ (20°C, Tomlin 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
2.69 × 10⁻⁴ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.75 (RP-HPLC-$k'$ correlation, Braumann et al. 1983)
- 3.43 (shake flask-GC, Ichmann et al. 1993)
- 2.06 to −0.22 (pH 4–7, shake flask-LSC, Riise & Salbu 1992)
- 1.77 (Tomlin 1994)
- 3.43 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:
- 1.36 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log $K_{OC}$:
- 2.23 (soil, calculated-S, Kenaga 1980)
- 2.05, 2.07, 1.70, 1.79, 1.73 (5 soils: soil A 30.4% OC and pH 4.4, soil B 14.6% OC pH 4.1, soil C/loam 3.3% OC pH 5.0, soil D/silty clay 1.3% OC pH 5.1, soil E/sand 1.4% OC pH 5.3, batch equilibrium-sorption isotherms, Riise Salbu 1992)
- 1.08–1.60 (Tomlin 1994)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Photolysis: photodegradation $t_{1/2} = 10$ to 19 d on 3 Spanish natural dry soils; $t_{1/2} = 22$ to 59 d on 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$–6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 16$–37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

Half-Lives in the Environment:
- Soil: $t_{1/2} = 12$ d and 8 d in Quachita Highlands = forest and grassland soil, respectively, $t_{1/2} = 10$ d in gross timbers forest soil, average $t_{1/2} = 10$ d in 3 soils (Altom & Stritzke 1973); selected field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996);
- $t_{1/2} \sim 8$ d in soil (Tomlin 1994)
- photodegradation $t_{1/2} = 10$–19 d in 3 Spanish natural dry soils, $t_{1/2} = 22$–59 d in the 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$–6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 16$–37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)
17.1.1.28 Diclofop-methyl

Common Name: Diclofop-methyl
Synonym: Hoelon, dichlordiphenoprop, Hoegrass, Illoxan
Chemical Name: methyl 2-[4-(2',4'-dichlorophenoxy)-phenoxy]propanoate
Uses: herbicide to control post-emergent wild oats, wild millets, and other annual grass weeds in wheat, barley, rye, red fescue, and broadleaf weeds in crops such as soybeans, sugar cane, fodder beet, flax, legumes, oilseed rape, sunflowers, clover, lucerne, groundnuts, brassicas, carrots, celery, beet root, parsnips, lettuce, spinach, potatoes, tomatoes, fennel, alliums, herbs, etc.
CAS Registry No: 51338-27-3
Molecular Formula: C_{16}H_{14}Cl_{2}O_{4}
Molecular Weight: 341.186
Melting Point (°C):
40 (Lide 2003)
Boiling Point (°C):
175–176 (at 0.1 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989)
Density (g/cm³):
1.035 (Herbicide Handbook 1989)
Acid Dissociation Constants, pKₐ:
3.1 (Wauchope et al. 1992; Hornsby et al. 1996)
Molar Volume (cm³/mol):
349.6 (calculated-Le Bas method at normal boiling point)
329.7 (calculated-density)
Dissociation Constant pHₐ:
3.1 (Wauchope et al. 1992; Hornsby et al. 1996)
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: 0.713 (mp at 40°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
3.0 (22°C, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)
3.0 (22°C, Herbicide Handbook 1989)
0.80 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.80 (20°C, pH 7, Tomlin 1994)
4.23 (Majewski & Capel 1995)
4.06 (calculated-group contribution method, Kühne et al. 1995)
3.0 (Lohninger 1994; Milne 1995)
0.8 (selected, Halfon et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
3.47 × 10⁻³, 1.6 × 10⁻⁴, 3.87 × 10⁻³ (20°C, 30°C, 54.3°C, Herbicide Handbook 1989)
5.91 × 10⁻³ (selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.5 × 10⁻³, 7.7 × 10⁻³ (20°C, 50°C, Tomlin 1994)
4.80 × 10⁻³ (quoted, Majewski & Capel 1987)
4.7 × 10⁻⁴ (selected, Halfon et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.00387 (calculated-P/C, Majewski & Capel 1995)
0.199 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{ow}$:
4.80 (shake flask, Log P Database, Hansch & Leo 1987)
4.601 (Stevens et al. 1988)
4.58 (Worthing & Hance 1991)
4.60 (shake flask, pH 7, Baker et al. 1992)
4.80 (recommended, Sangster 1993)
4.5775 (Tomlin 1994)
4.80 (recommended, Hansch et al. 1995)
5.52 (Pomona-database, Müller & Kördel 1996)
4.87 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF or log $K_B$:
2.74 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log $K_{OC}$:
4.69, 4.20 (Wauchope et al. 1992)
4.15–4.39 (soil, quoted values, Bottoni & Funari 1992)
4.25 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
4.15–4.39 (soil, Tomlin 1994)
4.20 (estimated-chemical structure, Lohninger 1994)
4.25; 3.61 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volutilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: first-order rate constants $k = -0.0883, -0.225, -0.266 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0158, -0.0139, -0.0134 \text{ h}^{-1}$ in sterile sediment by shake-tests at Davis Bayou, $k = -0.0457, -0.103, -0.120 \text{ h}^{-1}$ in nonsterile water and $k = -0.00233, -0.00722, -0.00785 \text{ h}^{-1}$ in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)
$t_{1/2} = 10 \text{ d}$ in sandy soils and $t_{1/2} \sim 30 \text{ d}$ in sandy clay soils under aerobic conditions (Herbicide Handbook 1989)
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} = 363 \text{ d}$ at 25°C and pH 5, $t_{1/2} = 31.7 \text{ d}$ at pH 7 and $t_{1/2} = 0.52 \text{ d}$ at pH 9 (Tomlin 1994).
Ground water: reported $t_{1/2} = 6–9, 23–38$ and 150 d (Bottoni & Funari 1992)
Sediment:
Soil: $t_{1/2} = 10 \text{ d}$ in sandy soils and $t_{1/2} \sim 30 \text{ d}$ in sandy clay soils while under anaerobic conditions, results were similar except that the very rapid cleavage of the ester bond by hydrolysis within one hour to propionic acid derivatives was experienced and within 2 d, up to 86% of the parent compound was metabolized into various free acid metabolites and up to 3.7% of phenol metabolites (Herbicide Handbook 1989);
\( t_{1/2} = 6–9 \text{ d, } 23–38 \text{ d and } 150 \text{ d (Bottoni & Funari 1992); } \\
\text{selected field } t_{1/2} = 30 \text{ d at pH 7.0 (Wauchope et al. 1992; Hornsby et al. 1996)} \\
V = 1–57 \text{ d and } t_{1/2} = 30–281 \text{ d for various soils in field trials (Tomlin 1994).} \\
\text{Biota: } t_{1/2} = 3–7 \text{ d for wheat (Herbicide Handbook 1989)} \\
\text{ } t_{1/2} = 3 \text{ d in sugar beet (Tomlin 1994).} \)
17.1.1.29 Dinitramine

Common Name: Dinitramine
Synonym: Cobex, Cobexo
Chemical Name: N,N-diethyl-2,6-dinitro-4-trifluoromethyl-m-phenylenediamine
Uses: herbicide for selective pre-plant soil incorporating control of many annual grass and broadleaf weeds in cotton, soybeans, peas, groundnuts, beans, sunflowers, safflowers, carrots, turnips, fennel, chicory, etc. and in transplanted tomatoes, capsicums, aubergines, and brassicas.
CAS Registry No: 29091-05-2
Molecular Formula: C₁₁H₁₃N₄O₄F₃
Molecular Weight: 322.241
Melting Point (°C): 98 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   265.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
   4.5 (Haag & Yao 1992)
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: 0.192 (mp at 98°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   1.0 (Wauchope 1978; Verschueren 1983)
   1.0 (20°C, Ashton & Crafts 1981; Hartley & Kidd 1987)
   1.1 (Worthing & Walker 1987, 1991)
   1.0 (20°C, Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
   0.00048 (Khan 1980; Ashton & Crafts 1981)
   0.00048 (Verschueren 1983)
   0.000479 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
   0.00040 (20°C, selected, Suntio et al. 1988)
   0.00048 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
   0.160 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log Kₐₜₜ:
   4.31 (selected, Dao et al. 1983)
   4.30 (Worthing & Hance 1991; Tomlin 1994)
   4.30 (Milne 1995)
   4.30 (recommended, Hansch et al. 1995)
   3.89 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Bioconcentration Factor, log BCF:
- 2.77 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 2.45 (calculated-$K_{OC}$, Kenaga 1980)

Sorption Partition Coefficient, log $K_{OC}$:
- 3.60 (soil, Harvey 1974)
- 3.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 3.84 (estimated-chemical structure, Lohninger 1994)
- 3.63 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 3.63; 3.42 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:
- Photolysis: $t_{1/2} < 1$ h in distilled water, river water and ocean water under sunlight (Newsom & Woods 1973; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 22$ d for 0.5 $\mu$g/mL to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:
- Soil: $t_{1/2} = 22$ d for 0.5 $\mu$g/mL to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991);
- persistence of 3 months in soil (Wauchope 1978);
- selected field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
- $t_{1/2} = 10–66$ d (Tomlin 1994).
17.1.1.30 Dinoseb

Common Name: Dinoseb  
Synonym: Anatox, Aretit, Basanite, Butaphene, Caldon, Chemox, Dibutox, Dinitral, DNBP, DN-289, DNOSAP, DNOSBP, DSNBP, Dow General, Dyanap, Dytop  
Chemical Name: 2-sec-butyl-4,6-dinitrophenol  
Uses: herbicides/insecticides; pre- or post-emergence control of broadleaf weeds in cereals, maize, lucerne, clover, trefoil, grass leys, potatoes, peas, onions, garlicks, peas, leeks, soya beans, orchards, groundnuts, strawberries, vineyards and other crops; for control of strawberry runners and raspberry suckers and overwintering forms of insect pests on fruit trees; also used as a desiccant for leguminous seed crops; destruction of potato haulms; as a pre-harvest hop defoliating, etc.

CAS Registry No: 88-85-7  
Molecular Formula: C\textsubscript{10}H\textsubscript{12}N\textsubscript{2}O\textsubscript{5}  
Molecular Weight: 240.212

Melting Point (°C):  
40  
(Le Bas 2003)

Boiling Point (°C):  
362  
(estimated, Grain 1982)

Density (g/cm\textsuperscript{3} at 20°C):  
1.265  
(45°C, Hartley & Kidd 1989; Milne 1995)

Molar Volume (cm\textsuperscript{3}/mol):  
218.0  
(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK\textsubscript{a}:  
4.62  
(radiometer/pH meter, Cessna & Grover 1978; Hornsby et al. 1996)

4.61  
(radiometer/pH meter, Cessna & Grover 1978)

4.62  
(Worthing & Walker 1987, 1991)

4.50  
(Yao & Haag 1991)

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: 0.713 (mp at 40°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):  
50  
(Günther 1968; Spencer 1982; Thomas 1982)

52  
(Kearney & Kaufman 1975; Khan 1980)

50  
(Martin & Worthing 1977; Kenaga 1980)

52  

100  

52  
(20°C, Hartley & Kidd 1987; Milne 1995)

52  
(20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):  
130  
(151.5°C, Khan 1980)

133  
(151.1°C, Ashton & Crafts 1981)

0.0008, 0.0067 (supercooled liquid, estimated, Grain 1982)

0.0067  
(Thomas 1982)

0.0023  
(30°C, Spencer 1982)

10  
(20°C, selected, Suntio et al. 1988)

0.183  
(60°C, Worthing & Hance 1991)

0.0067  
(20–25°C, selected, Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
51.1 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log $K_{ow}$:  
- 3.59 (Hansch & Leo 1979)  
- 3.69 (calculated, Zitko et al. 1976)  
- 3.69 (Hansch & Leo 1985)  
- 4.10 (RP-PHLC-RT correlation, Klein et al. 1988)  
- 3.0, 3.57 (pH 7, pH 2, shake flask, Brooke et al. 1990)  
- 3.69 (recommended, Sangster 1993)  
- 3.56 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:  
- 1.83 (calculated-S, Kenaga 1980a; quoted, Howard 1991)  
- 0.778 (calculated-$K_{oc}$, Kenaga 1980)  
- 1.51 (measured, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, log $K_{OC}$:  
- 2.85 (soil, Thomas 1982)  
- 2.09 (soil, Kenaga 1980a; Kenaga & Goring 1980)  
- 2.71 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980a)  
- 3.82 (HPLC-‘k’ correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)  
- 2.68 (estimated as log $K_{OM}$, Magee 1991)  
- 1.80, 2.04, 2.08 (soil, literature values, Bottoni & Funari 1992)  
- 2.70 (selected, Lohninger 1994)  
- 2.09 (soil, calculated-MCI 1′, Sabljic et al. 1995)  
- 1.48 (soil, 20–25°C, estimated, Hornsby et al. 1996)

Adsorption coefficient, $K_d$ (L·kg⁻¹):  
- 6.4, 64 (homoionic K⁺-kaolinite, K⁺-montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:  
Volatilization: initial rate constant $k = 1.1 \times 10^{-3}$ h⁻¹ and predicted rate constant $k = 2.6 \times 10^{-3}$ h⁻¹ from soil with $t_{1/2} = 266.5$ h (Thomas 1982).  
Photolysis: Oxidation:  
- photooxidation $t_{1/2} = 12.2–122$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)  
- $k(aq.) = \left(0.003–2\right) \times 10^5$ M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 1.9–5.0 and 24 ± 1°C, with $t_{1/2} = 0.16$ s at pH 7 (Yao & Haag 1991).  
- $k(calc) = 4 \times 10^9$ M⁻¹ s⁻¹ for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao 1992).  
Hydrolysis: Biodegradation: aqueous aerobic $t_{1/2} = 1032–2952$ h, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991) and aqueous anaerobic $t_{1/2} = 96–360$ h, based on anaerobic soil die-away test data for isopropalin (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991).  
Biotransformation:  
- Bioconcentration, Uptake ($k_1$) and Elimination Constants ($k_2$):  

Half-Lives in the Environment:  
Air: $t_{1/2} = 12.2–122$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).  
Surface water: $t_{1/2} = 1032–2952$ h, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);
measured rate constant $k = (0.003–2) \times 10^5 \text{ M}^{-1} \text{s}^{-1}$ for direct reaction with ozone in water at pH 1.9 -5.0 and 24 ± 1°C, with $t_{1/2} = 0.16 \text{ s}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 96–5904 \text{ h}$, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)
reported $t_{1/2} = 30 \text{ d}$ (Bottoni & Funari 1992)

Sediment:
Soil: $t_{1/2} = 1032–2952 \text{ h}$, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);
reported $t_{1/2} = 30 \text{ d}$ (Bottoni & Funari 1992);
field $t_{1/2} = 30 \text{ d}$ at 20–25°C (estimated, Hornsby et al. 1996).

Biota:
## 17.1.1.31 Diphenamid

![Chemical Structure of Diphenamid]

**Common Name:** Diphenamid  
**Synonym:** Difenamide, Dimid, Dymid, Enide, Fenam, Rideon  
**Chemical Name:** *N,N*-dimethyldiphenylacetamide; *N,N*-dimethyl-α-phenyl-benzeneacetamide  
**Uses:** herbicide for pre-emergence control of annual grasses and some broadleaf weeds in cotton, sweet potatoes, tomatoes, vegetables, capsicums, okra, soybeans, groundnuts, tobacco, pome fruit, stone fruit, citrus fruit, bush fruit, strawberries, forestry nurseries, and ornamental plants, shrubs, and trees.

**CAS Registry No:** 957-51-7  
**Molecular Formula:** C_{16}H_{17}NO  
**Molecular Weight:** 239.312  
**Melting Point (°C):** 135  
(Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):** 1.17  
(23.3 °C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)  
**Molar Volume (cm³/mol):** 284.2  
(calculated-Le Bas method at normal boiling point)  
**Dissociation Constant pK₁:**  
**Enthalpy of Fusion, ΔH₉₀ (kJ/mol):** 27.405  
(DSC method, Plato & Glasgow 1969)  
**Entropy of Fusion, ΔS₉₀ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS₉₀ = 56 J/mol K), F:** 0.0833  
(mp at 135°C)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):** 240  
(Melnikov 1971)  
260  
260  
(Martin & Worthing 1977; Weber et al. 1980; Kenaga 1980)  
260  
280  
(20–25°C, selected, Hornsby et al. 1996)  
**Vapor Pressure (Pa at 25°C or as indicated):** < 1.33 × 10⁻⁴  
(Weber et al. 1980)  
negligible  
(20°C, Hartley & Kidd 1987; Tomlin 1994)  
4.0 × 10⁻⁶  
(20–25°C, selected, Hornsby et al. 1996)  
**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):**  
**Octanol/Water Partition Coefficient, log K_{OW}:**  
**Bioconcentration Factor, log BCF:** 1.43  
(calculated-S, Kenaga 1980)  
**Sorption Partition Coefficient, log K_{OC}:** 2.32  
(soil, calculated-S, Kenaga 1980)  
2.32  
(selected, Lohninger 1994)  
2.32  
(soil, 20–25°C, selected, Hornsby et al. 1996)
Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:
  Photolysis: t₁/₂ = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

Half-Lives in the Environment:
  Soil: estimated persistence of 8 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);
    persistence under warm damp conditions is ca. 3–6 months (Herbicide Handbook 1989; Tomlin 1994)
    field t₁/₂ = 30 d at 20–25°C (selected, Hornsby et al. 1996).

Biota:
17.1.1.32 Diquat

Common Name: Diquat
Synonym: Aquacide, Deiquat, Dextrone, Ortho, Pathclear, Preeglone, Reglone, Weedol, Weedtrine-D
Chemical Name: 1,1′-ethylene-2,2′-dipyridine
Uses: nonselective contact herbicide to control broadleaf weeds in fruit and vegetable crops.
CAS Registry No: 2764-72-9
Molecular Formula: C_{12}H_{14}N_{2}
Molecular Weight: 186.236
Melting Point (°C): 335–340 (Spencer 1982)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
230.6 (calculated-Le Bas method at normal boiling point)
149.6 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entergy 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):
700000 (Khan 1980; Spencer 1982)
670000 (Weber et al. 1980)
700000 (Verschueren 1983)
700000 (Worthing & Hance 1991; Tomlin 1994)
700000 (Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
< 0.00533 (Agrochemicals Handbook 1983)
< 1.3 × 10⁻⁵ (Worthing & Hance 1991; Tomlin 1994)
< 1.3 × 10⁻⁵ (20°C, Montgomery 1993)
Henry’s Law Constant (Pa-m³/mol at 25°C or as indicated):
< 3.42 × 10⁻⁹ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow}:
−3.05 (Garten & Trabalka 1983)
2.78 (Reinert 1989)
−4.60 (20°C, Worthing & Hance 1991; Tomlin 1994)
−4.60 (Montgomery 1993)
Bioconcentration Factor, log BCF:
−2.84 (calculated-S as per Kenaga 1980, this work)
−5.92 (calculated-log K_{ow} as per Mackay 1982, this work)
Sorption Partition Coefficient, log K_{OC}:
2.84 (Reinert 1989)
0.420 (calculated, Montgomery 1993)
0.425 (calculated-S as per Kenaga 1980, this work)
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

**Vaporization:**
- $t_{1/2} = 192$ h for 10 µg/mL to degrade in distilled water under 240–260 nm light (Funderburk et al. 1960; quoted, Cessna & Muir 1991);
- $t_{1/2} < 5$ wk for 4 µg/mL to degrade in distilled water under sunlight (Slade & Smith 1967; quoted, Cessna & Muir 1991);
- dry diquat photodecomposed by UV light with $t_{1/2} = 48$ h (Funderburk & Bozarth 1967; quoted, Montgomery 1993);
- $t_{1/2} \sim 48$ h when associated with aerosols (Howard 1991);
- $t_{1/2} = 3$ wk for 3% of 5 µg/mL to degrade in distilled water under sunlight (Smith & Grove 1969; quoted, Cessna & Muir 1991).

**Photolysis:**
- $t_{1/2} = 192$ h for 10 µg/mL to degrade in distilled water under 240–260 nm light (Funderburk et al. 1960; quoted, Cessna & Muir 1991);
- $t_{1/2} < 5$ wk for 4 µg/mL to degrade in distilled water under sunlight (Slade & Smith 1967; quoted, Cessna & Muir 1991);
- dry diquat photodecomposed by UV light with $t_{1/2} = 48$ h (Funderburk & Bozarth 1967; quoted, Montgomery 1993);
- $t_{1/2} \sim 48$ h when associated with aerosols (Howard 1991);
- $t_{1/2} = 3$ wk for 3% of 5 µg/mL to degrade in distilled water under sunlight (Smith & Grove 1969; quoted, Cessna & Muir 1991).

**Oxidation:**
- $k(aq.) = 5.9 \times 10^9$ M$^{-1}$ s$^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
- $k(aq.) = (0.6 \pm 0.2)$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C, with a half-life of 15 h at pH 7 (Yao & Haag 1991).
- $k(aq.) = (8.0 \pm 1.8) \times 10^8$ M$^{-1}$ s$^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at 24 ± 1°C (Haag & Yao 1992).

**Hydrolysis:**
- $t_{1/2} = 74$ d under simulated sunlight at pH 7 (Montgomery 1993; Tomlin 1994).

**Biodegradation:**
- $t_{1/2} > 158$ d for 1.5 µg/mL of infested sediment-water microcosm to biodegrade (derived from results of Simsiman & Chesters 1976; Muir 1991).

**Biotransformation:**

**Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:**

**Half-Lives in the Environment:**

**Air:**
- Surface water: $t_{1/2} \sim 50$ d to biodegrade in lake water (Hiltibran 1972; quoted, Muir 1991);
- $t_{1/2} \sim 2$ d of $^{14}$C-diquat in water of a weed-infested simulated lake impoundment containing Lake Mendota sediment, the rapid disappearance is attributed to adsorption by sediments, suspended particulate matter and aquatic plants (shake flask-liquid scintillation spectrometry, Simsiman & Chesters 1976)
- measured rate constant $k = (0.6 \pm 0.2)$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C, with $t_{1/2} = 15$ h at pH 7 (Yao & Haag 1991).

**Ground water:**
- Sediment: Slow microbial degradation due to tight bonding of adsorbed Diquat to the clay minerals on the sediment (shake flask-liquid scintillation spectrometry, Simsiman & Chesters 1976)
- $t_{1/2} > 158$ d for 1.5 µg/mL of infested sediment-water microcosm to biodegrade (derived from results of Simsiman & Chesters 1976; Muir 1991).

**Soil:**

**Biota:**
17.1.1.33 Diuron

Common Name: Diuron
Synonym: AF 101, Cekiuron, Crisuron, Dailon, DCMU, Diater, dichlorofonidim, Di-on, Direx, DMU, Drexel, Duran, Dynex, Herbatox, Karmex, Marmer, NA 2767, Telvar, Unidron, Urox D, Vonduron
Chemical Name: 3-(3,4-dichlorophenyl)-1,1-dimethylurea; \(N\prime-(3,4\text{-dichlorophenyl})-N,N\text{-dimethylurea}\)
Uses: pre-emergence herbicide in soils to control germinating broadleaf grasses and weeds in crops such as apples, cotton, grapes, pears, pineapple, and alfalfa; also used as sugar cane flowering depressant.

CAS Registry No: 330-54-1
Molecular Formula: \(C_{9}H_{10}Cl_{2}N_{2}O\)
Molecular Weight: 233.093
Melting Point (°C):
158 (Lide 2003)
Boiling Point (°C):
180 (decomposes, Montgomery 1993)
Density (g/cm\(^3\) at 20°C):
Molar Volume (cm\(^3\)/mol):
223.8 (calculated-Le Bas method at normal boiling point)
188.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)
Dissociation Constant \(pK_{a}\):
–1 to –2 (Montgomery 1993)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
66.0 (Rordorf 1989)
Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
33.89 (DSC method, Plato & Glasgow 1969)
27.3 (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: 0.0496 (mp at 158°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
42.0 (Günther et al. 1968; Melnikov 1971; Spencer 1973, 1982; Khan 1980; Ashton & Crafts 1981)
42.0 (20°C, Weber 1972; Weber et al. 1980)
37.3 (shake flask-UV, Freed et al. 1976; Freed 1976)
42.4 (shake flask, Briggs 1981)
22.0 (shake flask-HPLC, Ellgehausen et al. 1981)
38.7 (generator column-HPLC/RI, Swann et al. 1983)
120 (RP-HPLC-RT correlation, Swann et al. 1983)
19.6, 40.1, 53.4 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
42.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
40.0 (20°C, Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.6 × 10\(^{-5}\) (estimated, Nex & Swezey 1954)
3.8 × 10\(^{-6}\) (20°C, Johnson & Julin 1974)
4.1 × 10\(^{-4}\) (50°C, Khan 1980; Ashton & Crafts 1981)
< 1.3 × 10\(^{-4}\) (20–25°C, Weber et al. 1980)
2.5 × 10\(^{-4}\) (Thomas 1982)
Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated):

- 1.4 × 10^{-4} (calculated-P/C, Jury et al. 1984, 1987a,b; Jury & Ghodrati 1989)
- 1.2 × 10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
- 1.3 × 10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
- 0.274 (calculated-P/C, Howard 1991)
- 2.1 × 10^{-5} (20°C, calculated-P/C, Muir 1991)
- 1.5 × 10^{-4} (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 2.60 (calculated-f const., Rekker 1977)
- 2.81 (Rao & Davidson 1980)
- 2.68 (shake flask-UV, Briggs 1981)
- 2.89 (shake flask-HPLC, Ellgehausen et al. 1981)
- 2.60 (Elgar 1983)
- 2.77 (Hansch & Leo 1985)
- 2.69, 2.65, 2.63 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
- 2.86 (shake flask, Mitsutake et al. 1986)
- 1.97–2.81 (Montgomery 1993)
- 2.78 (recommended, Sangster 1993)
- 2.45 (RP-HPLC-RT correlation, Sichballi & Finizio 1993)
- 2.80 (Aquasol Database 1994; quoted, Pinsuwan et al. 1995)
- 2.81 (shake flask, Spurlock & Biggar 1994a)
- 2.85 ± 1.70 (Tomlin 1994)
- 2.58, 2.73 (shake flask-UV, RP-HPLC-k’ correlation, Liu & Qian 1995)
- 2.68 (recommended, Hansch et al. 1995)
- 2.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log \( BCF \):

- 1.40 (measured, Isensee 1976)
- 1.88 (calculated-S, Kenaga 1980)
- 1.34 (calculated-\( K_{OC} \), Kenaga 1980)
- 2.16 (\textit{Pimephales promelas}, Call et al. 1987)
- 2.41, 2.48 (cuticle/water: tomato, pepper, Chaumat et al. 1991)
- 2.41, 2.51 (cuticle/water: box tree, laurel, Chaumat et al. 1991)
- 2.55, 2.28 (cuticle/water: pear, ivy, Chaumat et al. 1991)
- 1.18, 1.64 (cuticle/water: cleavers, vanilla, Chaumat et al. 1991)
- 2.45, 2.48 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Bioaccumulation Factor, log \( BF \):

- –1.70 (adipose tissue in both male & female Albino rats, Hodge et al. 1967)

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

- 2.60 (soil, Hamaker & Thompson 1972; Farmer 1976; Hance 1976)
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2.75 (soil, calculated-S as per Kenaga & Goring 1977, Kenaga 1980)
2.59 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.15–2.52 (Peck et al. 1980)
2.21 (soil, converted from reported $K_{OW}$ multiplied 1.724, Briggs 1981)
3.06, 2.41 (estimated-S, solubility and mp, Karickhoff 1981)
1.58, 2.42 (estimated-$K_{OW}$, Karickhoff 1981)
2.58 (average of 84 soils, Rao & Davidson 1982)
2.18 (soil, Thomas 1982)
2.83 (Webster soil, Nkedi-Kizza 1983)
2.49 (soil slurry method, Swann et al. 1983)
2.48 (RP-HPLC-RT correlation, Swann et al. 1983)
3.03, 2.94 (4°C, 25°C, Semiahmoo soil, batch equilibrium method-LSS, Madhun et al. 1986)
2.82, 2.68 (4°C, 25°C, Adkins soil, batch equilibrium method-LSS, Madhun et al. 1986)
2.86, 2.44, 2.48; 2.81, 2.74, 2.44 (estimated-$K_{OW}$; solubility, Madhun et al. 1986)
2.50 (calculated-MCI $\chi$, Gerstl & Helling 1987)
2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
2.35, 2.57 (2 subsurface soils from Oklahoma, Bouchard & Wood 1988)
2.94, 2.68 (mucky peat soil, loam sand soil, quoted, Howard 1991)
2.18, 2.48–2.49, 2.59, 2.66 (soil, quoted values, Bottoni & Funari 1992)
2.21–2.87 (Montgomery 1993)
2.68 (selected, Lohninger 1994)
2.60 (Tomlin 1994)
2.70 (calculated-$K_{OW}$, Liu & Qian 1995)
2.40 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
3.07, 2.37, 2.82, 2.51, 2.96 (calculated-$K_{OW}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.48, 2.42 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.44, 2.43, 2.57 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, 0.1 $\leq OC < 0.5\%$, average, Delle Site 2001)
2.78 (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

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

Volatilization: $2.5 \times 10^{-3}$ h⁻¹ (initial) and $5.3 \times 10^{-4}$ h⁻¹ (predicted) from soil with $t_\frac{1}{2} = 1307$ h (Thomas 1982; the calculated $t_\frac{1}{2} = 1918$ d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991).

Photolysis: $t_\frac{1}{2} = 2.25$ h for 80–84% of 40 $\mu$g/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991); in surface waters should be photolyzed within a few days (Howard 1991).

Oxidation: photooxidation $t_\frac{1}{2} = 0.12$ d in air, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Hydrolysis: $t_\frac{1}{2} > 4$ months for 4660 $\mu$g/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: $t_\frac{1}{2} = 328$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a); $t_\frac{1}{2} = 3–10$ d for 40 $\mu$g/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a quoted, Muir 1991); $t_\frac{1}{2} < 17$ d for 40 $\mu$g/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b; quoted, Muir 1991); 67–99% will be degraded in 10 wk under aerobic conditions by mixed cultures isolated from pond water and sediments forming 6–7 products (Ellis & Camper 1982; quoted, Howard 1991; Muir 1991); $t_\frac{1}{2} < 70$ d at 30°C (Ellis & Camper 1982; quoted, Muir 1991; Montgomery 1993); $t_\frac{1}{2} \sim 5$ d for 0.22 $\mu$g/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985; quoted, Muir 1991); $t_\frac{1}{2}(aerobic) \sim 20$ d for 0.0005–10 $\mu$g/mL to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).
Biotransformation: ~ 7% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of diuron (20 mg/L) in 5-d experiment (Vroumsia et al. 1996)

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

Half-Lives in the Environment:

Air: t½ = 0.12 d, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: should be photolyzed within a few days (Howard 1991).

Ground water: reported half-lives or persistence, t½ = 20–70, 90–180, 200, and 328 d (Bottoni & Funari 1992)

Sediment: t½ = 3–10 d for 40 µg/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a; quoted, Muir 1991);

< 17 d for 40 µg/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b);

≈ 5 d for 0.22 µg/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985)

Soil: estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

= 7.0 months at 15°C and = 5.5 months at 30°C in soils (Freed & Haque 1973);

persistence of 10 months (Wauchope 1978);

rate constant k = 0.0031 d⁻¹ with t½ = 328 d under field conditions (Rao & Davidson 1980);

calculated t½ = 1918 d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991);

≈ 200–4000 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

= 705, 414, and 225 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while t½ = 1392, 630, and 406 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives were considerable higher in peat. t½ = 3991, 2164, and 1165 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while t½ = 3416, 1832, and 896 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhum & Freed 1987)

t½ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

reported t½ = 20–70 d, 90–180 d, 200 d and 328 d (Bottoni & Funari 1992);

≈ 75–102 d in 0–40 cm soil cores taken, from cultivated field, t½ = 55–65 d from meadow and t½ = 29–35 d from gravel track (Hassink et al. 1994);

selected field t½ = 90 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical t½ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).
17.1.1.34 EPTC

Common Name: EPTC
Synonym: Eptam, Eradicane, FDA 1541, R 1608, Torbin
Chemical Name: carbamic acid, dipropylthio-, S-ethyl ester; S-ethyldipropyl(thiocarbamate); S-ethyldipropylcarbamo-thioate
Uses: selective systemic herbicide for pre-emergence control of perennial and annual grasses, broadleaf weeds.
CAS Registry No: 759-94-4
Molecular Formula: C₉H₁₉NOS
Molecular Weight: 189.318
Melting Point (°C): liquid
Boiling Point (°C):
- 235.0 (Khan 1980; Herbicide Handbook 1989)
- 127.0 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
- 236.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHᵢₕₜₕ (kJ/mol):
Entropy of Fusion, ΔSᵢₕₜₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSᵢₕₜₕ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 375 (shake flask-GC, Freed et al. 1967)
- 365 (Martin & Worthing 1977)
- 370–375 (Weber et al. 1980)
- 375 (20°C, Spencer 1982)
- 370 (Beste & Humburg 1983; Jury et al. 1983, 1984)
- 375 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
- 365 (20°C, Budavari 1989; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
- 4.666 (extrapolated, Patchett et al. 1964)
- 20.66 (Bailey & White 1965)
- 1.84 (20°C, effusion method, Hamaker & Kerlinger 1971)
- 2.16, 2.63, 3.69, 8.266 (23, 24, 28, 40°C, Hamaker 1972)
- 2.62 (20°C, volatilization rate, Burkhard & Guth 1981)
- 2.80 (Patchett et al. 1983)
- 0.612 (20°C, GC-RT correlation, Kim 1985)
- 4.70 (Hartley & Kidd 1987)
- 2.00 (20°C, selected, Suntio et al. 1988)
- 4.532 (35°C, Budavari 1989)
- 4.50 (Worthing & Hance 1991)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

- 1.32 (20°C, volatilization rate, Burkhard & Guth 1981)
- 1.02 (20°C, calculated-P/C, Suntio et al. 1988)
- 1.463 (calculated-P/C, Taylor & Glotfelty 1988)
- 1.023 (calculated-P/C, this work)

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

- 1.76 (selected, Dao et al. 1983)
- 3.21 (shake flask, Log P Database, Hansch & Leo 1987)
- 3.21 (recommended, Sangster 1993)
- 3.21 (recommended, Hansch et al. 1995)
- 3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.34 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 1.08 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

- 2.38 (soil, Hamaker & Thompson 1972)
- 2.45 (soil, Hamaker & Thompson 1972)
- 2.23 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 2.23–2.38, 2.45 (quoted values, Bottoni & Funari 1992)
- 2.30 (soil, 20–25°C, selected, Wauchope et al. 1992)
- 2.38 (Montgomery 1993)
- 2.30 (selected, Lohninger 1994)
- 2.45 (selected, Wienhold & Gish 1994)
- 2.38 (soil, calculated-MCI X, Sabljic et al. 1995)
- 2.23, 1.98 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.03, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

- Volatilization: t_{1/2} = 3.7 d (Jury et al. 1983).
- Photolysis: rate constant k = 5.2 × 10^{-5} s^{-1} for a light intensity corresponding to a 12-h average NO₂ photolysis rate with a black lamp spectral distribution (Kwok et al. 1992); photodegradation t_{1/2} = 14.0 and 18.5 min in water solution under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).
- Oxidation: second order rate constants k_{OH} = (3.10–3.40) × 10^{-11} cm³ molecule⁻¹ s⁻¹ for gas-phase reaction with OH radical, k_{NO₃} = 0.92 × 10^{-14} cm³ molecule⁻¹ s⁻¹ with NO₃ radical and k_{O₃} < 1.3 × 10^{-19} cm³ molecule⁻¹ s⁻¹ with O₃ at 298 K (Kwok et al. 1992); calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).
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Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetimes are: > 8 h due to photolysis, 5.8 d due to reaction with OH radical, 5.0 d with NO$_3$ radical and > 125 d with O$_3$ (Kwok et al. 1992);

Surface water: $t_{\text{½}} = 14.0$ and 18 min for elimination in water under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Ground water: reported half-lives or persistence, $t_{\text{½}} = 7$ and 30 d (Bottoni & Funari 1992)

Sediment:
Soil: estimated persistence of 4 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);
$t_{\text{½}} = 30$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
$t_{\text{½}} \sim 1$ wk in moist loam soil at 21 to 27°C (Herbicide Handbook 1974, 1989);
reported $t_{\text{½}} = 7$, 30 d (Bottoni & Funari 1992);
selected field $t_{\text{½}} = 6$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical $t_{\text{½}} = 30$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989)
17.1.1.35 Ethalfluralin

Common Name: Ethalfluralin
Synonym: Benzenamine, Somilan, Sonalan, Sonalen
Chemical Name: N-ethyl-N-(2-methyl-2-propenyl)-2.6-dinitro-(trifluoromethyl)-benzenamine
CAS Registry No: 55283-68-6
Uses: herbicide
Molecular Formula: C₁₃H₁₄F₃N₃O₄
Molecular Weight: 333.263
Melting Point (°C):
  57  (Lide 2003)
Boiling Point (°C):
  256  (decomposes, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₖₑ₅ (kJ/mol):
Entropy of Fusion, ΔSₖₑ₅ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₖₑ₅ = 56 J/mol K), F: 0.485 (mp at 57°C)
Water Solubility (g/m³ or mg/L at 25°C):
  0.21  (Ashton & Crafts 1981)
  0.20  (pH 7, Spencer; Hartley & Kidd 1987; Worthing & Walker 1987)
  0.30  (pH 7, Herbicide Handbook 1989)
  0.30  (selected, Wauchope et al. 1992; Hornsby et al. 1996)
  0.30  (pH 7, Tomlin 1994; Milne 1995)
  0.40  (Majewski & Capel 1995)
Vapor Pressure (Pa at 25°C or as indicated):
  1.10 × 10⁻⁴  (Worthing & Walker 1983, 1987; Hartley & Kidd 1987)
  0.0109  (Spencer 1982; Herbicide Handbook 1989)
  0.0117  (selected, Wauchope et al. 1992; Hornsby et al. 1996)
  0.0117  (Tomlin 1994)
  2.22 × 10⁻⁴  (20–25°C, Majewski & Capel 1995)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  0.183  (calculated-P/C, Majewski & Capel 1995)
  13  (calculated-P/C, Wolt 1997)
Octanol/Water Partition Coefficient, log Kₐₖₗ:
  5.11  (pH 7, Tomlin 1994; Milne 1995)
  4.92  (quoted values; selected, Wolt 1997)
Octanol/Air Partition Coefficient, log Kₐₐ:
Bioconcentration Factor, log BCF or log Kₐₐ:
Herbicides

Sorption Partition Coefficient, log $K_{oc}$:
- 3.60 (selected, soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.60–3.90 (soil, Tomlin 1994)
- 3.61–3.92 (soil, Wolt 1997)

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

Volatilization:
- Photolysis: $t_\frac{1}{2} = 6.3$ h in aqueous phase and $t_\frac{1}{2} = 2$ h in vapor phase (Tomlin 1994);
  - Aqueous photolysis $t_\frac{1}{2} = 6.3$ h in pH 5 sterile buffer solution; soil photolysis $t_\frac{1}{2} = 14.2$ d in air-dry sandy loam soil when exposed to a xenon light source; air photolysis $t_\frac{1}{2} = 2$ h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Oxidation:
- Hydrolysis: no hydrolysis after 33 d at pH 3, 6 and 9 (51°C, Tomlin 1994); stable in sterile, buffered solutions across a range of pH (Wolt 1997).

Biodegradation:
- Biotransformation: $t_\frac{1}{2} = 45$ d for aerobic metabolism in sandy loam soils and $t_\frac{1}{2} = 14$ d for more rapid metabolism anaerobically in the same soil (quoted, Tomlin 1994; Wolt 1997).

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

Half-Lives in the Environment:
- Air: air photolysis $t_\frac{1}{2} = 2$ h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).
- Surface water: water photolysis $t_\frac{1}{2} = 6.3$ h in pH 5 sterile buffer solution; $t_\frac{1}{2} = 2$ d for dissipation from the water column in a pond water-sediment system under outdoor conditions (Wolt 1997).
- Ground water:
  - Sediment: $t_\frac{1}{2} = 38$ h in anaerobic pond water-sediment system (Wolt 1997).
  - Soil: reported field $t_\frac{1}{2} = 30–60$ d, 60 d, 25–46 d; recommended $t_\frac{1}{2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);
    - $t_\frac{1}{2} = 45$ d for aerobic metabolism in sandy loam soils and $t_\frac{1}{2} = 14$ d for more rapid metabolism anaerobically in the same soil (Tomlin 1994);
    - Terrestrial field dissipation $t_\frac{1}{2} = 4–146$ d, $t_\frac{1}{2} = 45$ d in moist aerobic soil, $t_\frac{1}{2} = 14$ d in anaerobic soil shifted to anaerobic conditions (Wolt 1997).
- Biota:
17.1.1.36  Fenoprop

Chemical Name: 2-(2,4,5-trichlorophenoxy) propionic acid

Common Name: Fenoprop
Synonym: Silvex, 2,4,5-TP, Kuron, Kurosal, Fruitone T

Molecular Formula: C₉H₇Cl₃O₃
Molecular Weight: 269.509

Melting Point (°C):
181.6 (Lide 2003)

Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
2.84 (Worthing 1983, 1987; Augustijn-Beckers et al. 1994)

Enthalpy of Vaporization, ΔHv (kJ/mol):
75.75 (Rordorf 1989)

Enthalpy of Fusion, ΔHfus (kJ/mol):
44.6 (Rordorf 1989)

Entropy of Fusion, ΔSfus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
0.0291 (mp at 181.6°C)

Water Solubility (g/m³ or mg/L at 25°C):
140 (Kenaga & Goring 1980, Kenaga 1980a,b, Spencer 1982)
140 (Worthing & Walker 1983, 1987; Budavari 1989)
200 (Verschueren 1983)
176 (Hartley & Kidd 1987)
12.0 (calculated-MCI χ, Patil 1994)
140 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.30 × 10⁻³, 4.40 × 10⁻², 0.55, 4.90, 34.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pa) = 13.953 − 4948/(T/K); measured range 85.4–181°C (gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pa) = 11.727 − 3956.9/(T/K); measured range 181–211°C (gas saturation-GC, Rordorf 1989)
< 1.33 × 10⁻⁶ (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log Kow:
2.44 (Kenaga 1980a)
3.86 (estimated, Garten & Trabalka 1983)
3.13 (counter-current chromatography, Ilchmann et al. 1993)
2.75 (calculated-MCI χ, Patil 1994)
3.80 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Koa:

Bioconcentration Factor, log BCF or log Kbi:
1.76 (calculated, Kenaga 1980a)
1.58, 2.23 (calculated-solubility, Kow, Kenaga 1980b)
Herbicides

1.76  (fish, flowing water, Garten & Grabalka 1983)
2.35  (Isensee 1991)

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

3.41  (soil, Kenaga & Goring 1980)
2.46  (calculated-$K_{ow}$, Kenaga 1980b)
1.91  (soil: calculated-MCI $\chi$, Meylan et al. 1992)
2.48  (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28  (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

Biodegradation: $t_{1/2} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983)

Half-Lives in the Environment:

Soil: persistence 47–205 d in soil (Alexander et al. 1961)

degradation $t_{1/2} = 21$ d and 14 d in Quachita Highlands’ forest and grassland soil respectively, $t_{1/2} = 15$ d in gross timbers forest soil, average $t_{1/2} = 17$ d in 3 soils (Altom & Stritzke 1973);

$t_{1/2} = 5–11$ d in a microagroecosystem study (Nash 1983);

$t_{1/2} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983);

field $t_{1/2} = 21$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
17.1.1.37 Fenuron

Common Name: Fenuron
Synonym: Dozer, Dybar, Falisilvan, Fenidim, Fenulon, Urab
Chemical Name: 1,1-dimethyl-3-phenylurea; $N,N^\prime$-dimethyl-$N^\prime$-phenylurea
Uses: herbicide to control woody plants and deep-rooted perennial weeds, often used in combination with chlorpropham to extend its weed control spectrum and range of crops.
CAS Registry No: 101-42-8
Molecular Formula: $C_9H_{12}N_2O$
Molecular Weight: 164.203
Melting Point (°C):
132 (Lide 2003)
Boiling Point (°C):
Density (g/cm$^3$ at 20°C):
1.13 (25°C, Hartley & Kidd 1987)
1.08 (Worthing & Hance 1991; Tomlin 1994)
Molar Volume (cm$^3$/mol):
182.0 (calculated-Le Bas method at normal boiling point)
159.0 (modified Le Bas method, Spurlock & Biggar 1994a)
Dissociation Constant $pK_a$:
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
24.267 (DSC method, Plato & Glasgow 1969)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0892 (mp at 132°C)
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
2600 (Freed 1966)
2400 (Günther et al. 1968)
3850 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Verschueren 1983)
3850 (Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)
3700 (shake flask-HPLC, Ellgehausen et al. 1981)
3000 (20°C, selected, Suntio et al. 1988)
3900 (Spurlock 1992; Spurlock & Biggar 1994b)
Vapor Pressure (Pa at 25°C or as indicated):
0.0213 (60°C, Khan 1980; Verschueren 1983)
0.0210 (60°C, Hartley & Kidd 1987)
0.0050 (20°C, selected, Suntio et al. 1988)
0.0210 (60°C, Worthing & Hance 1991; Tomlin 1994)
0.0267 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C at 25°C or as indicated):
0.00027 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log $K_{ow}$:
0.98 (shake flask-UV, Hansch & Anderson 1967)
1.00 (Leo et al. 1971)
1.00 (shake flask-UV, Lord et al. 1980)
Herbicides

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.96</td>
<td>(shake flask-UV, Briggs 1981; Karickhoff 1981)</td>
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<tr>
<td>0.88</td>
<td>(shake flask-HPLC, Ellgehausen et al. 1981)</td>
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<td>0.62</td>
<td>(HPLC-(k') correlation, McDuffie 1981)</td>
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<tr>
<td>0.70</td>
<td>(Elgar 1983)</td>
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<tr>
<td>1.18</td>
<td>(RP-HPLC-(k') correlation, Braumann et al. 1983)</td>
</tr>
<tr>
<td>1.00</td>
<td>(shake flask-HPLC, Spurlock &amp; Biggar 1994a)</td>
</tr>
<tr>
<td>0.98</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>1.18</td>
<td>(RP-HPLC-RT correlation, Sicbaldi &amp; Finizio 1993)</td>
</tr>
<tr>
<td>0.98</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>1.18</td>
<td>(RP-HPLC-RT correlation, Finizio et al. 1997)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

- 0.778 (calculated-S, Kenaga 1980)
- 0.0 (calculated-K\(\text{OC}\), Kenaga 1980)
- 1.34 (earthworms, Lord et al. 1980)
- 0.699, 0.602 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K\(\text{OC}\):

- 1.43 (soil, Hamaker & Thompson 1972)
- 1.67 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 0.88 (reported as log K\(\text{OM}\), Briggs 1981)
- 0.61 (estimated-K\(\text{OW}\), Karickhoff 1981)
- 1.80, 1.86 (estimated-S, Karickhoff 1981)
- 0.72, 0.84 (estimated-S and \(\text{mp}\), Karickhoff 1981)
- 1.74 (calculated-MCI \(\chi\), Gerstl & Helling 1987)
- 1.40 (soil, calculated-MCI \(\chi\), Sabljic et al. 1995)
- 1.40; 1.40, 1.70 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 1.42, 1.41 (soils: organic carbon \(\text{OC} \geq 0.1\%\), \(\text{OC} \geq 0.5\%\), average, Delle Site 2001)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_\text{½}\):

Biodegradation: aerobic \(t_\text{½} \geq 10\ d\) for 0.01 \(\mu g/mL\) to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991).

Half-Lives in the Environment:

- Air:
  - Surface water: aerobic \(t_\text{½} \geq 10\ d\) for 0.01 \(\mu g/mL\) to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);
  - persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971).
- Ground water:
- Sediment:
- Soil: \(t_\text{½} = 4.5\) months at 15°C and 2.2 months at 30°C in soils (Freed & Haque 1973);
  - persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
  - selected field \(t_\text{½} = 60\ d\) (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:
17.1.1.38 Fluchloralin

Common Name: Fluchloralin
Synonym: BAS-392H, Basalin
Chemical Name: \( N-(2\text{-chloroethyl})-2,6\text{-dinitro-}N\text{-propyl-}4\text{-trifluoromethyl}\text{benzenamine}; N-(2\text{-chloroethyl})\alpha,\alpha,\alpha\text{-trifluoro-}
2,6\text{-dinitro-}N\text{-propyl-p-toluidine} \)
Uses: herbicide for pre-plant or pre-emergence control of annual grass and broadleaf weeds in cotton, groundnuts, jute, potatoes, rice soybeans, and sunflowers, etc.

CAS Registry No: 33245-39-5
Molecular Formula: \( C_{12}H_{13}ClF_{3}N_{3}O_{4} \)
Molecular Weight: 355.697
Melting Point (°C):
42 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
326.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant \( pK_a \):
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: 0.681 (mp at 42°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1.00 (20°C, Weber 1972; Ashton & Crafts 1981)
1.00 (Edwards 1977)
0.70 (20°C, Spencer 1982)
< 1.0 (Worthing & Walker 1987, 1991; Tomlin 1994)
10 (Budavari 1989; Milne 1995)
0.90 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.50 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
0.0033 (20°C, Weber 1972; Worthing & Walker 1987)
0.373 (20°C, Ashton & Crafts 1981)
0.0008, 0.0033, 0.0133, 0.533 (20, 30, 40, 50°C, gas saturation, Spencer 1982)
0.0035 (Herbicide Handbook 1983; quoted, Nash 1988)
0.0037, 0.0033 (20°C, 30°C, Herbicide Handbook 1989)
0.004 (20°C, Worthing & Hance 1991; Tomlin 1994)
0.004 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.174 (20°C, calculated-P/C, Muir 1991)
1.343 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
4.63 (selected, Magee 1991)
Bioconcentration Factor, log BCF:

> 2.79, 2.40 (calculated-S, calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.56  (soil, Harvey 1974)
3.60  (soil, Kenaga 1980)
> 3.64  (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.25  (calculated-MCI \chi, Bahnick & Doucette 1988)
3.56; 3.58  (reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
3.80  (estimated-chemical structure, Lohninger 1994)
3.55  (soil, calculated-MCI \chi, Sabljic et al. 1995)
3.55; 4.02  (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatileization: estimated t_{1/2} ~ 1 d from 1 m depth of water (20°C, Muir 1991).

Photolysis: t_{1/2} = 13 d for 84% of 5 µg/mL to degrade in distilled water under sunlight (Nilles & Zabik 1974; quoted, Cessna & Muir 1991);

Oxidation:

Hydrolysis:

Biodegradation: t_{1/2} = 8 d for 0.5 µg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:

Half-Lives in the Environment:

Soil: t_{1/2} = 8 d for 0.5 µg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

t_{1/2} = 1.5 d on Bosket silt loam, t_{1/2} = 4 d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with t_{1/2} = 13 d on Bosket silt loam, t_{1/2} = 8 d on Sharkey clay (Savage & Jordan 1980)

measured dissipation rate k = 0.099–0.13 d^{-1} (derived from Savage & Jordan 1980, Nash 1988);

field studies, t_{1/2} = 12.2 wk - 1978 first study; t_{1/2} = 13.0 wk -1978 second study; t_{1/2} = 17.6 wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

Laboratory studies: t_{1/2} = 28.7 wk at 4°C, 10.5 wk at 25°C for soils of field capacity moisture (27% w/w for Crowley silt loam) and t_{1/2} = 20.8 wk at 4°C, t_{1/2} = 8.4 wk at 25°C for flooded soil of Crowley silt loam;

t_{1/2} = 29.3 wk at 4°C, t_{1/2} = 10.5 wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay) and t_{1/2} = 20.8 wk at 4°C and t_{1/2} = 4.3 wk at 25°C for flooded soil, Sharkey silty clay (Brewer et al. 1982);

t_{1/2} = 3.6 wk for 2.0 µg/mL to biodegrade in soil at 25°C (derived form Brewer et al. 1982, Muir 1991);

estimated dissipation rate k = 0.29, and 0.120 d^{-1} (Nash 1988);

estimated field t_{1/2} ~ 60 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
17.1.1.39 Fluometuron

Common Name: Fluometuron
Synonym: CIBA 2059, Cotoran, Cottonex, Higalcoton, Lanex, Meturon, Pakhtaran
Chemical Name: 1,1-dimethyl-3-(α,α,α-trifluoro-m-tolyl)urea; N,N-dimethyl-N′-[3-(trifluoromethyl)phenyl]urea
Uses: herbicide to control many annual broadleaf weeds in sugar cane and cotton.
CAS Registry No: 2164-17-2
Molecular Formula: C_{10}H_{11}F_{3}N_{2}O
Molecular Weight: 232.201
Melting Point (°C):
164 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm⁢³/mol):
229.7 (calculated-Le Bas method at normal boiling point)
167.1 (calculated-density)
Dissociation Constant pKₐ:
–1.00 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
29.706 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0433 (mp at 164°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
90 (20°C, Martin & Worthing 1977; Herbicide Handbook 1978,89)
106 (shake flask-UV, Briggs 1981)
90 (Herbicide Handbook 1983)
80 (Montgomery 1993)
110 (Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
6.70 × 10⁻⁵ (20–25°C, Weber et al. 1980)
6.70 × 10⁻⁵ (Herbicide Handbook 1983)
6.60 × 10⁻⁵ (20°C, Worthing & Hance 1991)
1.25 × 10⁻⁴ (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
< 0.283 (20–25°C, calculated-P/C, Montgomery 1993)
1.73 × 10⁻⁴ (calculated-P/C, this work)
Herbicides

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 1.34 (Briggs 1969)
- 2.42 (shake flask-UV, Briggs 1981)
- 1.88 (shake flask-UV, pH 5, Barak et al. 1983)
- 2.40 (selected, Gerstl & Helling 1987)
- 2.23 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 2.23, 2.38 (Montgomery 1993)
- 2.03 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.20 (recommended, Sangster 1993)
- 2.42 (recommended, Hansch et al. 1995)
- 2.03 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
- 1.67 (calculated-S, Kenaga 1980)
- 0.954 (calculated-$K_{OC}$, Kenaga 1980)

Sorption Partition Coefficient, log $K_{OC}$:
- 2.24 (soil, Abernethy & Davidson 1971; Davidson & McDougal 1973; Savage & Wauchope 1974; Carringer et al. 1975; Wood & Davidson 1975)
- 2.30 (soil, Kenaga 1980)
- 2.57 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.82 (soil, converted from reported $K_{OW}$ multiplied by 1.724, Briggs 1981)
- 2.30 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 1.46–2.08 (Montgomery 1993)
- 2.00 (estimated-chemical structure, Lohninger 1994)
- 1.49–2.07 (Tomlin 1994)
- 2.00 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.33; 2.66, 2.03, 2.64, 2.36, 1.94 (quoted lit., calculated-$K_{OW}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.14, 2.51 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:
Photolysis: $t_\text{1/2} = (11 \pm 2)$ h in 10 ppm aqueous solutions under summer sunlight of 9.1 h/d exposure and $t_\text{1/2} = (33 \pm 16)$ h under spring sunlight of 3.7 h/d exposure (Burkhard et al. 1975).

Oxidation:
Hydrolysis: $t_\text{1/2} = 1.6$ yr at 20°C and pH 1, $t_\text{1/2} = 2.4$ yr at pH 5, and $t_\text{1/2} = 2.8$ yr at pH 9 (Montgomery 1993).

Biodegradation:
Biotransformation:

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

Half-Lives in the Environment:

Air:
Surface water: $t_\text{1/2} = 730–1010$ d at pH 5–9 and 20°C in aqueous solutions (Herbicide Handbook 1989).

Ground water:

Sediment:
Soil: measured dissipation rate $k = 0.023–0.043$ d$^{-1}$ (Horowitz & Herzlinger 1974; quoted, Nash 1988);
estimated dissipation rate $k = 0.0012$, and 0.011 d$^{-1}$ (Nash 1988);
persistence of 4 months in soil (Wauchope 1978);
selected field $t_\text{1/2} = 85$ d (Wauchope et al. 1992; Hornsby et al. 1996);
soil $t_\text{1/2} = 30$ d (Pait et al. 1992);
median $t_\text{1/2} \sim 30$ d in soil (Herbicide Handbook 1989; Tomlin 1994).

Biota:
17.1.1.40 Fluorodifen

Common Name: Fluorodifen
Synonym: Preforan, Soyex
Chemical Name: 4-nitrophenyl α,α,α-trifluoro-2-nitro-p-tolyl ether
Uses: herbicide.
CAS Registry No: 15457-05-3
Molecular Formula: C_{13}H_{7}F_{3}N_{2}O_{5}
Molecular Weight: 328.200
Melting Point (°C):
94 (Spencer 1982; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
282.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 0.210 (mp at 94°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
2.0 (20°C, Spencer 1973, 1982)
< 2.0 (Weber et al. 1980)
2.0 (shake flask-HPLC, Ellgehausen et al. 1981)
2.0 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)
Vapor Pressure (Pa at 25°C or as indicated):
9.33 × 10⁻⁶ (20°C, Spencer 1982)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
3.30 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)
4.40 (20 ± 2°C, shake flask-UV, Briggs 1981)
3.65 (shake flask-HPLC, Ellgehausen et al. 1981)
3.60 (HPLC-RT correlation, Nandihalli et al. 1993)
3.65 (recommended, Sangster 1993)
3.65 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
2.019 (algae, log BF-bioaccumulation factor, Ellgehausen et al. 1980)
2.386 (catfish, log BF-bioaccumulation factor, Ellgehausen et al. 1980)
1.178 (daphnids, log BF-bioaccumulation factor, Ellgehausen et al. 1980)
Sorption Partition Coefficient, log K_{OC}:
3.13 (calculated-MCI χ, Gerstl & Helling 1987)
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Half-Lives in the Environment:
17.1.1.41 Fluridone

Common Name: Fluridone
Synonym: Brake, EL-171, Fluridon, Pride, Sonar
Chemical Name: 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl] 4(1H)-pyridinone; 1-methyl-3-phenyl-5-(α,α,α-trifluoro-m-tolyl)-4-pyridone
Uses: herbicide to control annual grass and broadleaf weeds and certain perennial species in cotton; also used to control aquatic weeds and plants in lakes, ponds, ditches, etc.
CAS Registry No: 59756-60-4
Molecular Formula: C_{19}H_{14}F_{3}NO
Molecular Weight: 329.315
Melting Point (°C): 155 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
333.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant: 12.3 (pKₐ, Wauchope et al. 1992)
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: 0.0530 (mp at 155°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
12.0 (20°C, Weber 1972; Worthing & Walker 1987)
12.0 (Kenaga 1980)
12.0 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)
10.0 (selected, Lohninger 1994)
Vapor Pressure (Pa at 25°C or as indicated):
1.31 × 10⁻³ (20°C, Weber 1972; Worthing & Walker 1987)
1.00 × 10⁻³ (Herbicide Handbook 1983)
0.013 (Hartley & Kidd 1987; Worthing & Hance 1991)
1.33 × 10⁻³ (Herbicide Handbook 1989)
1.30 × 10⁻³ (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
3.59 × 10⁻⁴ (20°C, calculated-P/C, Muir 1991)
Octanol/Water Partition Coefficient, log K_{ow}:
1.87 (Reinert 1989)
1.87 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.98 (shake flask, Takahashi et al. 1993; quoted, Sangster 1993)
3.16 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Bioconcentration Factor, log BCF:
2.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
0.778 (measured, West et al. 1983; quoted, Isensee 1991)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
1.60 (soil, Kenaga 1980)
2.97–3.39 (pond sediment, Muir et al. 1980)
3.36, 2.95 (lake and river sediment, Muir et al. 1980)
2.94 (Reinert 1989)
2.90, 3.81, 3.03 (Norfolk sand pH 6.0, Norfolk with montmorillonite pH 5.9, Norfolk sand with added organic matter pH 5.3, Reinert 1989)
3.43, 2.57, 2.43 (California soil at pH 6, 7, 7.3, Reinert 1989)
3.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (selected, Lohninger 1994)
2.85 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatile: estimated $t_{1/2} = 10,000$ d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: $t_{1/2} \sim 23$ h to degrade in distilled water under > 290 nm light (West et al. 1979; quoted, Cessna & Muir 1991);
$u = 6$ h for 5 $\mu$g/mL to degrade in nonsterile pond water under sunlight (Muir & Grift 1982; quoted, Cessna & Muir 1991);
$u = 27$ d for 85% of 10 $\mu$g/mL to degrade in distilled water and for 85% of 10 $\mu$g/mL to degrade in lake water at pH 8.4 both under sunlight (Sanders & Mosier 1983; quoted, Cessna & Muir 1991; Howard et al. 1991)
resistance to decomposition by UV light with $u = 23$ h in deionized water (Herbicide Handbook 1989).
Hydrolysis: $u > 113$ d for 1 $\mu$g/mL to hydrolyze in pond water at 4°C (Ghassemi et al. 1981; quoted, Muir 1991); $u = 23$ h in water (Tomlin 1994).
Biodegradation: aqueous aerobic $u = 44–192$ d, based on soil die-away test data and field study soil persistence (Banks et al. 1979; quoted, Howard et al. 1991);
$u = 12$ months for 5 $\mu$g/mL to biodegrade in static sediment and water, and $u = 9$ months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991);
aqueous anaerobic $u = 176$ d to 2.1 yr, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
microbial degradation $u > 343$ d at pH 7.3 with 2.6% organic matter in a silt loam soil (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 0.9–1.3$ h$^{-1}$ (Chironomus tentans larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
$k_1 = 0.70–5.6$ h$^{-1}$ (Chironomus tentans larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
$k_1 = 1.7–3.40$ h$^{-1}$ (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
$k_1 = 1.7–2.1$ h$^{-1}$ (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)
$k_2 = 0.052$ h$^{-1}$ (Chironomus tentans larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)
$k_2 = 0.118$ h$^{-1}$ (Chironomus tentans larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)
$k_2 = 0.055$ h$^{-1}$ (Chironomus tentans larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)
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k₂ = 0.041 h⁻¹ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:


Surface water: t₀₂ ~ 21 d in water (Hartley & Kidd 1987);
- t₀₂ = 288–864 h, based on estimated photolysis half-life in water (Howard et al. 1991);
- anaerobic t₀₂ = 9 months and aerobic t₀₂ ~ 20 d (Tomlin 1994).

Ground water: t₀₂ = 2112–9216 h, based on estimated unacclimiated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: t₀₂ = 12 months for 5 µg/mL to biodegrade in static sediment and water, and t₀₂ ~ 9 months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991).

Soil: measured dissipation rate k = 0.0041 d⁻¹ (Banks et al. 1979; quoted, Nash 1988) with estimated t₀₂ = 44–192 d (Banks et al. 1979; quoted, Howard et al. 1991);
- estimated dissipation rate k = 0.0067 and 0.025 d⁻¹ (Nash 1988);
- selected field t₀₂ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996);
- t₀₂ ~ 90 d in the hydrosol (Tomlin 1994).

Biota: elimination t₀₂ = 13.2 h in pond sediment-water, t₀₂ = 5.9 h in river water, t₀₂ = 12.5 h in river sediment-water, t₀₂ = 16.9 in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)
### 17.1.1.42 Glyphosate

Common Name: Glyphosate  
Synonym: Mon-0573, 0468, 2139; Polado, Roundup  
Chemical Name: $N$-(phosphoromethyl)glycine  
Uses: nonselective, post-emergent, broad spectrum herbicide to control annual and perennial grasses, sedges, broadleaf, and emerged aquatic weeds; also used to control insects on fruit trees.

CAS Registry No: 1071-83-6  
Molecular Formula: $\text{C}_3\text{H}_8\text{NO}_5\text{P}$  
Molecular Weight: 169.074  
Boiling Point (°C):  
Density (g/cm³ at 20°C): 1.74 (Herbicide Handbook 1989; Montgomery 1993)  
Molar Volume (cm³/mol):  
Dissociation Constant $pK_a$:  
5.70 (Worthing & Hance 1991)  
2.60, 5.90, 10.40 (pK₁, pK₂, pK₃, Yao & Haag 1991; Haag & Yao 1992)  
2.32, 5.86, 10.86 (pK₁, pK₂, pK₃, Montgomery 1993; Hornsby et al. 1996)  
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: 0.0097 (mp at 230°C)

Water Solubility (g/m³ or mg/L at 25°C):  
15700 (Herbicide Handbook 1989)  
12000 (Budavari 1989; Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):  
$2.59 \times 10^{-5}$ (45°C, Herbicide Handbook 1989)  
$4.00 \times 10^{-5}$ (Worthing & Hance 1991)  
0.001 (Montgomery 1993; quoted, Majewski & Capel 1995)  
negligible (Tomlin 1994)  
0.0 (selected, Halfon et al. 1996)

Henry’s Law Constant (Pa m³/mol at 25°C):  
$1.41 \times 10^{-3}$ (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:  
$-1.70$ (shake flask, pH 5.3, Martin & Edgington 1981)  
$-4.10$ (shake flask, pH 2.5, Stevens et al. 1988)  
$-3.25$ (Reinert 1989)  
$-4.59$ (Worthing & Hance 1991)  
$-1.60$ (Montgomery 1993)  
$-4.10, -1.70$ (pH 2.5, pH 5.3, quoted, Sangster 1993)  
$-1.70$ (pH 5.3, selected, Hansch et al. 1995)  
0.94 (RP-HPLC-RT correlation, Finizio et al. 1997)
Bioconcentration Factor, log BCF:

- 0.477 \ (\text{calculated-S, Kenaga 1980; quoted, Isensee 1991})
- 2.26 \ (\text{calculated-K_{OC}, Kenaga 1980})

Sorption Partition Coefficient, log K_{OC}:

- 3.42 \ (\text{soil, Sprankle et al. 1975; Hance 1976; Nomura & Hilton 1977})
- 1.40 \ (\text{soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980})
- 1.22 \ (\text{selected, USDA 1989; quoted, Neary et al. 1993})
- -0.43 \ (\text{Reinert 1989})
- 3.69, 3.53, 3.42 \ (3 \text{agricultural soils: Houston clay loam at pH 7.5, Muskingum silt loam at pH 5.8, Sassafras sandy loam at pH 5.6, Reinert 1989})
- 4.38 \ (\text{organic carbon, Wauchope et al. 1991})
- 3.43–3.69 \ (\text{Montgomery 1993})

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

**Vaporization:**

- Photolysis: \( t_{\frac{1}{2}} = 48 \text{ h for } 0\% \text{ of } 168 \mu g/mL \text{ to degrade in distilled water under } > 290 \text{ nm light (Rueppel et al. 1977; quoted, Cessna & Muir 1991);}
- \( t_{\frac{1}{2}} = 9 \text{ wk for } > 90\% \text{ of } 2 \mu g/mL \text{ to degrade in distilled water under sunlight (Lund-Hoie & Friestad 1986; quoted, Cessna & Muir 1991);}
- \( t_{\frac{1}{2}} = 4.0 \text{ d and } 3–4 \text{ wk for aqueous solutions of } 1.0 \text{ and } 2000 \text{ ppm under indoor UV light (Lund-Hoie & Friestad 1986; quoted, Montgomery 1993).}

**Oxidation:**

- \( k(aq.) = 7.3 \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at } 24 \pm 1^\circ \text{C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992);}
- \( k(aq.) = (0.027–8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 1.8–7.0 and } 22 \pm 2^\circ \text{C, with a half-life of } 4.0 \text{ s at pH 7 (Yao & Haag 1991).}
- \( k(aq.) = (1.8 \pm 0.5) \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at } 24 \pm 1^\circ \text{C (Haag & Yao 1992).}

**Hydrolysis:**

- \( t_{\frac{1}{2}} = 7 \text{ d for } 10 \mu g/mL \text{ to hydrolyze in sterile water + soil (Rueppel et al. 1977; quoted, Muir 1991);}
- \( t_{\frac{1}{2}} = 32 \text{ d for } 25 \text{ and } 250 \mu g/mL \text{ to hydrolyze in sterile distilled water at pH 3, 6 and 9 in the dark at } 5 \text{ and } 35^\circ \text{C (Ghassemi et al. 1981; quoted, Muir 1991).}

**Biodegradation:**

- \( t_{\frac{1}{2}} < 28 \text{ d for } 10 \mu g/mL \text{ to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991);}
- \( t_{\frac{1}{2}} > 9 \text{ wk for } 2 \mu g/mL \text{ to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);}
- \text{rate constant } k = 0.1 \text{ d}^{-1} \text{ from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);}
- \( t_{\frac{1}{2}} = 70 \text{ d in pond water at pH 7.2, } t_{\frac{1}{2}} = 63 \text{ d in swamp water at pH 6.3 and } t_{\frac{1}{2}} = 49 \text{ d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991).}

**Biotransformation:**

- **Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:**

Half-Lives in the Environment:

**Air:**

- Surface water: \( t_{\frac{1}{2}} > 9 \text{ wk for } 2 \mu g/mL \text{ to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);}
- \( t_{\frac{1}{2}} = 70 \text{ d in pond water at pH 7.2, } t_{\frac{1}{2}} = 63 \text{ d in swamp water at pH 6.3 and } t_{\frac{1}{2}} = 49 \text{ d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991);}
- \text{measured rate constant } k = (0.027 - 8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 1.8–7.0 and } 22 \pm 2^\circ \text{C, with } t_{\frac{1}{2}} = 4.0 \text{ s at pH 7 (Yao & Haag 1991).}

**Ground water:**

- Sediment:
Soil: $t_{\text{soil}} < 28$ d for 10 $\mu$g/mL to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991); estimated first-order $t_{\text{soil}} = 7$ d from biodegradation rate constant $k = 0.1$ d$^{-1}$ from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982); moderately persistent in soil with $t_{\text{soil}} = 20–100$ d (Willis & McDowell 1982); average $t_{\text{soil}} < 60$ d (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993); selected $t_{\text{soil}} = 47$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993; Halton et al. 1996).

Biota: average $t_{\text{soil}} = 60$ d in the forest (USDA 1989; quoted, Neary et al. 1993).
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17.1.1.43 Isopralin

Common Name: Isopralin
Synonym: EL 179, Isopraline, Isopralin solution, Paarlan
Chemical Name: 4-isopropyl-2,6-dinitro-N,N-dipropylaniline; 4-(1-methylethyl)-2,6-dinitro-N,N-dipropylbenzenamine;
2,6-dinitro-N,N-dipropylcumidine
Uses: herbicide used pre-planting and incorporated with soil preparation to control broadleaf weeds and grasses in
transplanted tobacco, and in direct-seeded tomatoes and capsicums.
CAS Registry No: 33820-53-0
Molecular Formula: C15H23N3O4
Molecular Weight: 309.362
Melting Point (°C): liquid
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
361.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₜₐₙ (kJ/mol):
Entropy of Fusion, ΔSₜₐₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₐₙ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.11 (Martin & Worthing 1977; Herbicide Handbook 1978)
1.10 (Ashton & Crafts 1981)
0.10 (Spencer 1982; Hartley & Kidd 1987; Budavari 1989; Milne 1955)
0.10 (Worthing & Walker 1987, Worthing & Hance 1991)
0.08 (Herbicide Handbook 1989)
0.10 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.02 (predicted-AQUAFAC, Lee et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
0.0019 (30°C, Ashton & Crafts 1981)
0.0019 (30°C, Hartley & Kidd 1987)
0.0040 (25.6°C, Herbicide Handbook 1989)
0.0012 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
5.34 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₐₜₐₙ:
Bioconcentration Factor, log BCF:
3.50 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
3.88 (calculated-K dư, Kenaga 1980)
Sorption Partition Coefficient, log K₊ₒᶜ:
4.88 (soil, Harvey 1974)
4.17 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.17–4.88 (soil, quoted values, Bottoni & Funari 1992)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization:
Photolysis: atmosphere photolysis t½ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis t½ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation t½ = 0.743–74.3 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:
Abiotic Transformation: Degradation by abiotic reductive transformations:

- k = 1.71 M⁻¹ s⁻¹ in H₂S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
- Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:
  - k = 0.94 × 10⁻³ h⁻¹ at pH 6.5, k = 0.36 × 10⁻² h⁻¹ at pH 7.0, k = 0.057 h⁻¹ at pH 7.4, and k = 1.76 h⁻¹ at pH 7.8 for aqueous ferrous ion system;
  - k = 0.297 h⁻¹ at pH 6.5, k = 0.586 h⁻¹ at pH 6.7, k = 1.28 h⁻¹ at pH 7.0, and k = 6.90 h⁻¹ at pH 7.3 for Fe(II)/goethite system;
  - k = 9.91 × 10⁻³ h⁻¹ at pH 6.5, k = 8.45 × 10⁻³ h⁻¹ at pH 7.0, k = 7.45 × 10⁻³ h⁻¹ at pH 7.4 and k = 6.96 × 10⁻² h⁻¹ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Biodegradation:
t½(aq. aerobic) = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)
t½(aq. anaerobic) = 96–360 h, based on anaerobic soil die-away test that tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air: t½ = 0.743–74.3 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: t½ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Ground water: t½ = 96–5040 h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991) reported t½ < 180 d (Bottoni & Funari 1992)

Sediment:

Soil: t½ = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);
selected field t½ = 100 d (Wauchope et al. 1992; Hornsby et al. 1996);

Biota:
17.1.1.44 Isoproturon

Common Name: Isoproturon
Synonym: Alon, Arelon, CGA 18731, Gramion, Graminon, Hoe 16410, Hytane, IP 50, IP flo, Tolkan
Chemical Name: 3-(4-isopropylphenyl)-1,1-dimethylurea; 3-p-cumenyl-l-1-dimethylurea
Uses: herbicide used for pre- and post-emergence control of annual grasses and broadleaf weeds in spring and winter wheat (except durum wheat), spring and winter barley, winter rye, and triticale.
CAS Registry No: 34123-59-6
Molecular Formula: C_{12}H_{18}N_{2}O
Molecular Weight: 206.284
Melting Point (°C):
- 155–156 (Worthing & Hance 1991)
- 158 (Tomlin 1994)
Boiling Point (°C):
Density (g/cm³ at 20°C):
- 1.16 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm³/mol):
- 259.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₚₕ (kJ/mol):
Entropy of Fusion, ΔSₚₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₕ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 60 (Martin & Worthing 1977)
- 70 (20°C, Spencer 1982)
- 72 (20°C, Hartley & Kidd 1987)
- 55.9 (Chaumat et al. 1991)
- 65 (20°C, selected, Traub-Eberhard et al. 1994)
Vapor Pressure (Pa at 25°C or as indicated):
- 3.3 × 10⁻⁶ (20°C, Spencer 1982; Hartley & Kidd 1987)
- 3.3 × 10⁻⁶ (20°C, Worthing & Hance 1991)
- 3.3 × 10⁻⁶, 3.15 × 10⁻³, 0.172 (20, 77, 150°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 1.05 × 10⁻³ (calculated-P/C, Otto et al. 1997)
- 1.24 × 10⁻³ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow} at 25°C or as indicated:
- 2.87 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.25 (Worthing & Hance 1991)
- 2.30 (shake flask, pH 7, Baker et al. 1992)
- 2.537 (calculated, Evelyne et al. 1992)
- 2.30 (Behrendt & Bruggemann 1993)
- 2.87 (recommended, Sangster 1993)
- 2.87 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
- 1.79 (calculated-S, Kenaga 1980)
- 1.76, 1.82 (cuticle/water: tomato, pepper; Chaumat et al. 1991)
- 1.71, 1.90 (cuticle/water: box tree, pear; Chaumat et al. 1991)
- 1.52, 1.20 (cuticle/water: ivy, vanilla; Chaumat et al. 1991)
- 1.76, 1.82 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, log $K_{OC}$:
- 2.66 (soil, calculated-S, Kenaga 1980)
- 1.86 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
- 2.11 (soil, quoted from Kördel et al. 1993, Traub-Eberhard et al. 1994)
- 1.86; 2.40 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.57, 1.71, 1.78, 1.73, 2.34 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.86, 2.31; 2.81, 2.24, 2.83, 2.35, 1.93 (quoted lit., calculated-$K_{OW}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 1999)
- 1.78, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

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

Volatilization:
- Photolysis: atmosphere photolysis $t_{1/2} = 288–864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);
- aqueous photolysis $t_{1/2} = 288–864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);
- $t_{1/2} = 1.5$ h for 215 µg/mL to degrade in distilled water under 254 nm light (Kulshrestha & Mukerjee 1986; quoted, Cessna & Muir 1991).

Oxidation: photooxidation $t_{1/2} = 0.743–74.3$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:
- Biodegradation: aqueous aerobic $t_{1/2} = 408–2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96–360$ h, based on anaerobic soil die-away test which tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)
- Biotransformation: ~ 11% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of isoproturon (100 mg/L) in 5-d experiment (Vroumsia et al. 1996)

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

Half-Lives in the Environment:
- Air: $t_{1/2} = 0.743–74.3$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
- Surface water: $t_{1/2} = 288–864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).
- Groundwater: $t_{1/2} = 96–5040$ h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)
- reported half-lives or persistence, $t_{1/2} = 12–29$ and 60–120 d (Bottoni & Funari 1992)
Sediment:
Soil: $t_{1/2} = 408–2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);
reported $t_{1/2} = 12–29$ d and 60–120 d (Bottoni & Funari 1992);
$t_{1/2} = 15–21$ d in sandy loam, $t_{1/2} = 11$ d in silt loam at 20°C (Traub-Eberhard et al. 1994)
Degradation and mineralization $t_{1/2} = 16$ d, 24 d and 34 d for pelosol, brown calcareous soil and brown acid soil, respectively, over 120 days under controlled laboratory conditions (Pieuchot et al. 1996)
estimated $t_{1/2} \sim 14.6$ d under conventional tillage, $t_{1/2} = 7.99$ d under ridge tillage and $t_{1/2} = 12.17$ d with no tillage (Otto et al. 1997).
17.1.1.45 Linuron

Common Name: Linuron
Chemical Name: 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea; \(N'-(3,4\text{-dichlorophenyl})-N\text{-methoxy}\text{-}N\text{-methylurea}\)

Uses: selective pre-emergence and post-emergence herbicide used on a wide variety of food crops to control many annual broadleaf and grass weeds.

CAS Registry No: 330-55-2
Molecular Formula: \(C_9H_{10}Cl_2N_2O_2\)
Molecular Weight: 249.093
Melting Point (°C): 93 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
232.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
90.23 (Rordorf 1989)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
28.66 (DSC method, Plato & Glasgow 1969)
25.9 (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: 0.215 (mp at 93°C)

Water Solubility (g/m³ or mg/L at 20°C or as indicated):
75 (Woodford & Evans 1963; Bailey & White 1965; Hartley & Graham-Bryce 1980; Kenaga 1980; Kenaga & Goring 1980; Beste & Humburg 1983)
81 (Hartley & Kidd 1987; Milne 1995)
81 (24°C, Worthing & Hance 1991)
75–81 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00147 (20°C, Quellette & King 1977)
0.0012 (20°C, Hartley & Graham-Bryce 1980)
0.002 (24°C, Khan 1980)
0.002 (20–25°C, Weber et al. 1980)
0.002 (24°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
0.0014 (20°C, selected, Suntio et al. 1988)
3.50 \times 10^{-4}, 1.10 \times 10^{-2}, 0.22, 2.90, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
\log (P_v/Pa) = 16.074 – 5824.2/(T/K); measured range 40.5–92 7°C (solid, gas saturation-GC, Rordorf 1989)
\log (P_v/Pa) = 12.989 – 4713.7/(T/K); measured range 92.7–160°C (liquid, gas saturation-GC, Rordorf 1989)
0.0011 (20°C, selected, Taylor & Spencer 1990)
0.0023 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
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<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C)</td>
<td>0.0027 (selected, Halfon et al. 1996)</td>
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<tr>
<td>Octanol/Water Partition Coefficient, log K_{ow}</td>
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<td></td>
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<tr>
<td>2.19</td>
<td>(Briggs 1969)</td>
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<tr>
<td>3.20</td>
<td>(shake flask-UV, Erkell &amp; Walum 1979)</td>
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<tr>
<td>2.76</td>
<td>(shake flask-UV, Briggs 1981)</td>
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<td>3.11</td>
<td>(shake flask, Mitsutake et al. 1986)</td>
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<td>2.48</td>
<td>(selected, Gerstl &amp; Helling 1987)</td>
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<td>3.00</td>
<td>(Worthing &amp; Hance 1991; Milne 1995)</td>
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<td>2.19, 3.00</td>
<td>(Montgomery 1993)</td>
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<td>2.75</td>
<td>(RP-HPLC-RT correlation, Sicbaldi &amp; Finizio 1993)</td>
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<td>(recommended, Sangster 1993)</td>
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<td>3.20</td>
<td>(recommended, Hansch et al. 1995)</td>
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<td>3.18</td>
<td>(Pomona-database, Müller &amp; Kördel 1996)</td>
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<td>2.75</td>
<td>(RP-HPLC-RT correlation, Finizio et al. 1997)</td>
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<td>2.72</td>
<td>(RP-HPLC-RT correlation, Yu et al. 1997)</td>
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<td>Bioconcentration Factor, log BCF:</td>
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<tr>
<td>1.73</td>
<td>(calculated-S, Kenaga 1980; quoted, Isensee 1991)</td>
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<tr>
<td>1.68</td>
<td>(calculated-K_{oc}, Kenaga 1980)</td>
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<tr>
<td>1.73</td>
<td>(calculated, Pait et al. 1992)</td>
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<td>Sorption Partition Coefficient, log K_{oc}:</td>
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<td>2.91</td>
<td>(soil, Hamaker &amp; Thompson 1972)</td>
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<td>2.61</td>
<td>(soil, calculated-S as per Kenaga &amp; Goring 1980, Kenaga 1980)</td>
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<td>2.93</td>
<td>(average soils/sediments, Rao &amp; Davidson 1980)</td>
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<td>2.43</td>
<td>(soil, converted form reported K_{oc} multiplied by 1.724, Briggs 1981)</td>
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<td>2.93, 2.80, 1.80</td>
<td>(estimated-S, calculated-S and mp, calculated-K_{oc}, Karickhoff 1981)</td>
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<td>3.83</td>
<td>(Means &amp; Wijayaratne 1982)</td>
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<td>2.99, 2.58; 2.62, 2.80</td>
<td>(estimated-K_{oc}, S, Madhun et al. 1986)</td>
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<td>2.76, 2.64</td>
<td>(quoted, calculated-MCI χ, Gerstl &amp; Helling 1987)</td>
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<td>2.94</td>
<td>(screening model calculations, Jury et al. 1987b)</td>
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<td>2.61–2.91, 2.83, 2.93</td>
<td>(soil, quoted values, Bottini &amp; Funari 1992)</td>
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<td>2.60</td>
<td>(soil, 20–25°C, selected, Wauchope et al. 1992;)</td>
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<td>2.70–2.78</td>
<td>(Montgomery 1993)</td>
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<td>2.59</td>
<td>(soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a)</td>
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<td>2.59</td>
<td>(soil, HPLC-screening method, Kördel et al. 1993, 1995b)</td>
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<td>2.70</td>
<td>(soil, calculated-MCI χ, Sablje et al. 1995)</td>
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<td>2.59; 2.54</td>
<td>(HPLC-screening method; calculated-PCKOC fragment method, Müller &amp; Kördel 1996)</td>
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<td>2.884, 2.58, 2.45, 1.33, 3.18</td>
<td>(second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)</td>
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<td>2.70; 2.55, 2.61</td>
<td>(soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)</td>
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<tr>
<td>2.65, 2.64</td>
<td>(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)</td>
<td></td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

Volatilization:
Photolysis: \( t_{1/2} = 2 \) months for 31\% of 55 \( \mu \)g mL\(^{-1} \) to degrade in distilled water under sunlight (Rosen et al. 1969; quoted, Cessna & Muir 1991);
\( t_{1/2} = 2.25 \) h for 67–75\% of 75 \( \mu \)g mL\(^{-1} \) to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
amosphere photolysis \( t_{1/2} = 1344–4032 \) h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis \( t_{1/2} = 1344–4032 \) h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation \( t_{1/2} = 0.49–4.90 \) h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: \( t_{1/2} > 4 \) months for 4980 \( \mu \)g mL\(^{-1} \) to hydrolyze in phosphate buffer at pH 5–9 and 20\(^\circ\)C (El-dib & Aly 1976; quoted, Muir 1991).

Biodegradation: \( t_{1/2} = 78 \) d in soil (Moyer et al. 1972; quoted, Means et al. 1983),
\( t_{1/2} = 87 \) d in soil (Hance 1974; quoted, Means et al. 1983),
\( t_{1/2} = 58 \) and 180 d in soil (Urosol & Hance 1974; quoted, Means et al. 1983);
aqueous aerobic \( t_{1/2} = 672–4272 \) h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);
rate constant \( k = 0.0096 \) d\(^{-1} \) by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
aqueous aerobic \( t_{1/2} \sim 40 \) d for 1 \( \mu \)g mL\(^{-1} \) to biodegrade in lake sediment and \( t_{1/2} \sim 60 \) d for 4 \( \mu \)g mL\(^{-1} \) to biodegrade in lake sediment and water (Huber & Gemes 1981; quoted, Muir 1991);
aqueous aerobic \( t_{1/2} \sim 20 \) d for 0.22 \( \mu \)g mL\(^{-1} \) to biodegrade in pond sediment plus aerobic salts medium of 34 g L\(^{-1} \) (Stepp et al. 1985; quoted, Muir 1991);
aqueous anaerobic \( t_{1/2} = 2688–17088 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
degradation rate constant \( k = (3.48 \pm 0.156) \times 10^{-2} \) d\(^{-1} \) with \( t_{1/2} = 19.9 \) d in control soil and \( k = (23.2 \pm 2.07) \times 10^{-2} \) d\(^{-1} \) with \( t_{1/2} = 2.99 \) d in pretreated soil in the field; \( k = (3.73 \pm 0.208) \times 10^{-2} \) d\(^{-1} \) with \( t_{1/2} = 18.6 \) d in control soil and \( k = (18.8 \pm 2.76) \times 10^{-2} \) d\(^{-1} \) with \( t_{1/2} = 3.68 \) d in pretreated soil once only in the laboratory (Walker & Welch 1991)

Biotransformation:
Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:

Air: \( t_{1/2} = 0.49–4.90 \) h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: \( t_{1/2} = 672–4272 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: \( t_{1/2} = 1344–8544 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
reported half-lives or persistence, \( t_{1/2} = 38–69 \) and 75 d (Bottoni & Funari 1992).

Sediment: degradation \( t_{1/2} = 12 \) d in estuarine sediment (12%/w) system (Cunningham et al. 1981; quoted, Means et al. 1983);
degradation \( t_{1/2} = 6 \) d in estuarine sediment (18%/w) system (Means et al. 1983).

Soil: estimated persistence of 4 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
\( t_{1/2} = 672–4272 \) h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);
persistence of 4 months (Wauchope 1978);
correlated $t_{1/2} = 57$ d at pH 5.1–5.8, $t_{1/2} = 22$ d at pH 6.3–7.0 and $t_{1/2} = 19$ d at pH 7.7–8.2 (Boddington Barn soil, Hance 1979) and $t_{1/2} = 67$ d at pH 4.6–5.2, $t_{1/2} = 53$ d at pH 5.3–6.1, and $t_{1/2} \sim 20$ d at pH 6.3–8.0 (Triangle soil, Hance 1979);

estimated first-order $t_{1/2} = 72$ d from biodegradation rate constant $k = 0.0096$ d$^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

decomposition $t_{1/2} = 11$ d in fresh soil and $t_{1/2} = 12$ d in air dried soil both in polyethylene bags, $t_{1/2} = 49$ d in undisturbed cores and $t_{1/2} = 40$ d in perfusion (Hance & Haynes 1981);

moderately persistent in soil with $t_{1/2} = 20–100$ d (Willis & McDowell 1982);

$t_{1/2} = 2$ to 5 months under field conditions (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);

$t_{1/2} = 75$ d from screening model calculations (Jury 1987b);

t$_{1/2} = 60, 35, 30$ d in plots treated, i.e., repeated application of pesticide, for the first, second, third and fourth time, respectively, in the field; in the laboratory $t_{1/2}$ reduced from 19 d to 3–7 d in a single pretreatment in moist oil at 20°C (Walker & Welch 1991)

reported $t_{1/2} = 38–69$ d and 75 d (Bottoni & Funari 1992);

selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 60$ d (Pait et al. 1992);

soil $t_{1/2} = 29–67$ d (Di Guardo et al. 1994).

Biota: biochemical $t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987b).
17.1.1.46 MCPA

Common Name: MCPA

Chemical Name: (4-chloro-2-methylphenoxy)acetic acid; 4-chloro-o-tolyloxyacetic acid

Uses: systemic post-emergence herbicide to control annual and perennial weeds in cereals, rice, flax, vines, peas, potatoes, asparagus, grassland and turf.

CAS Registry No: 94-74-6

Molecular Formula: C₉H₉ClO₃
Molecular Weight: 200.618

Melting Point (°C): 120 (Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
211.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:
3.05 (potentiometric titration, Nelson & Faust 1969)
3.125 (Cessna & Grover 1978)
3.07 (Worthing & Hance 1991)
3.05–3.13 (Montgomery 1993)
3.12 (Hornsby et al. 1996)

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: 0.117 (mp at 120°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1605 (shake flask-UV, Leopold et al. 1960)
1605 (Bailey & White 1965)
< 1000 (Khan 1980)
630 (20°C, Melnikov 1971)
825 (Martin & Worthing 1977; Weber et al. 1980; Milne 1995)
1500 (selected, Seiber et al. 1986)
825 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)
817 (selected, Gerstl & Helling 1987)
835 (room temp., Worthing & Walker 1987)
730–825 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
7.9 × 10⁻⁴ (measured-volatilization rate, Seiber et al. 1986)
2.0 × 10⁻⁴ (20°C, Hartley & Kidd 1987)
2.0 × 10⁻⁴ (21°C, Worthing & Walker 1987, 1991)
2.3 × 10⁻⁵ (20°C, Tomlin 1994)
2.0 × 10⁻⁴ (20°C, Milne 1995)
2.0 × 10⁻⁴ (selected, Halfon et al. 1996)
Henry’s Law Constant (Pa·m^3/mol at 25°C):

- $1.0 \times 10^{-4}$ (calculated-P/C, Seiber et al. 1986)
- $4.86 \times 10^{-4}$ (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- $< 0.010$ (estimated, Mabury & Crosby 1996)
- $2.5 \times 10^{-4}$ (calculated-P/C, this work)

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

- 2.69 (selected, Dao et al. 1983)
- 2.30 (RP-HPLC-$k'$ correlation, Braumann et al. 1983)
- 1.41 (selected, Gerstl & Helling 1987)
- 0.57 (shake flask-UV, pH 7, Stevens et al. 1988)
- 3.25 (countercurrent LC, Illchmann et al. 1993)
- 1.37–1.43 (calculated, Montgomery 1993)
- 0.57, 3.25 (quoted, Sangster 1993)
- 2.68 (MedChem Master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 1.15 (calculated-S, Kenaga 1980)

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

- 2.04 (soil, calculated-S, Kenaga 1980; quoted, Bottoni & Funari 1992)
- 1.95 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 2.03–2.07 (calculated, Montgomery 1993)
- 1.73 (calculated-QSAR MCI $\chi$, Sabljic et al. 1995)
- 2.49; 1.58, 3.27, 3.17, 1.85, 2.19 (calculated-$K_{ow}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)

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

Volatilization: $k = 9.78 \times 10^{-7}$ h$^{-1}$ at pH 3.5 (Seiber et al. 1986).

Photolysis: $t_{1/2} = 71$ h for $< 10\%$ of 50 $\mu$g mL$^{-1}$ to degrade in NaOH solution at pH 9.8 under $> 290$ nm light (Soderquist & Crosby 1975; quoted, Cessna & Muir 1991);
- $t_{1/2} = 245$ h for 17–98.5% of 9 $\mu$g mL$^{-1}$ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991);
- $t_{1/2} = 4.6$ d for 14,700 $\mu$g mL$^{-1}$ to degrade in droplets of spray solution suspended in air under sunlight (Freiberg & Crosby 1986; quoted, Cessna & Muir 1991).

Oxidation: degradation by ozone in dilute aqueous solutions (Benoit-Guyod et al. 1986) as follows:-
- $t_{1/2} = 9.4$ min - dark with $O_3$ in air; $t_{1/2} = 8.4$ min - light with $O_3$ in air; $t_{1/2} = 500$ min - light, air only, at initial pH of 3.55; MCPA concn of 224 $\mu$M L$^{-1}$, ozone input at 246 $\mu$M h$^{-1}$;
- $t_{1/2} = 10.4$ min - dark with $O_3$ in air; $t_{1/2} = 9.0$ min - light with $O_3$ in air, at initial pH of 8.0,
- $t_{1/2} = 11.5$ min - dark with $O_3$ in air; $t_{1/2} = 11.3$ min - light with $O_3$ in air, at initial pH of 7.0,
- $t_{1/2} = 8.4$ min - dark with $O_3$ in air; $t_{1/2} = 9.4$ min - light with $O_3$ in air, at initial pH of 7.0,
- $t_{1/2} = 4.2$ min - dark with $O_3$ in air; $t_{1/2} = 4.2$ min - light with $O_3$ in air, $t_{1/2} = 150$ min - light, air only, at initial pH of 8.0; MCPA concn of 5 $\mu$M L$^{-1}$, ozone input at 246 $\mu$M h$^{-1}$;
- $t_{1/2} = 176$ min - dark with $O_3$ in air; $t_{1/2} = 63$ min - light with $O_3$ in air, at initial pH of 8.0, MCPA concn of 224 $\mu$M L$^{-1}$, ozone input at 4.6 $\mu$M h$^{-1}$;
- $t_{1/2} = 300$ min - dark with $O_3$ in air; $t_{1/2} = 162$ min - light with $O_3$ in air, at initial pH of 8.0; MCPA concn of 224 $\mu$M L$^{-1}$, ozone input at 0.2 $\mu$M h$^{-1}$ (Benoit-Guyod et al. 1986).

Hydrolysis:

Biodegradation: $t_{1/2} > 168$ h for 1 $\mu$g mL$^{-1}$ to degrade in activated sludge (Schmidt 1975; quoted, Muir 1991); aerobic $t_{1/2} = 9$ d for 1 $\mu$g mL$^{-1}$ to degrade in natural water in absence of sunlight (Soderquist & Crosby 1975; quoted, Muir 1991);
- $t_{1/2} > 12$ d for 0.045–0.156 $\mu$g mL$^{-1}$ to degrade in water after application to model crop and washoff (Virtanen et al. 1979; quoted, Muir 1991);
t_{1/2} = 15–25 d for 10 µg mL\(^{-1}\) to degrade in flooded soils (Duah-Yentumi & Kuwatsuka 1980; quoted, Muir 1991);

first order microbial degradation \(k = 0.01393\) d\(^{-1}\) with \(t_{1/2} = 50\) d at room temp, \(k = 0.01687\) d\(^{-1}\) with \(t_{1/2} = 41\) d at 35°C in sandy clay soil from Finland; \(k = 0.02999\) d\(^{-1}\) with \(t_{1/2} = 23\) d at room temp, \(k = 0.03397\) d\(^{-1}\) with \(t_{1/2} = 20\) d at 35°C in sandy loam soil from Bangladesh (Sattar & Paasivirta 1980)

\(t_{1/2} > 25\) d for 10 µg mL\(^{-1}\) to degrade in flooded soils (Ursin 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: dissipation \(t_{1/2} \sim 4\) d in rice field; \(t_{1/2} = 17\) d in dilute aqueous solution under laboratory irradiation (Soderquist & Crosby 1975);

degradation \(t_{1/2} = 4.2 - 300\) min by ozone and light (UV > 300 nm) in dilute aqueous solution, depending on pH, concn of MCPA and ozone (shake flask-GC, Benoit-Guyod et al. 1986)

degraded rapidly with \(t_{1/2} = 9\) d in rice paddy water held under darkened conditions (Muir 1991)

field dissipation \(t_{1/2} = 28.8\) h in water (Mabury & Crosby 1996)

Ground water: reported \(t_{1/2} < 7\) and \(t_{1/2} = 20–25\) d (Bottoni & Funari 1992)

Sediment: \(t_{1/2} = 80\) to 400 d of MCPA at low concentrations in marine sediments (Muir 1991).

Soil: degradation \(t_{1/2} = 50\) d at room temp., \(t_{1/2} = 41\) d at 35°C in Finland sandy clay soil; degradation \(t_{1/2} = 23\) d at room temp., \(t_{1/2} = 20\) d at 35°C in Bangladesh loam soil from first-order rate constant obtained by linear regression (Sattar & Paasivirta 1980);

persistence of 3 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

\(t_{1/2} = 25\) d in flooded soils (Muir 1991);

\(t_{1/2} = 15\) d (selected, Halfon et al. 1996).

Biota:
17.1.1.47 MCPB

Common Name: MCPB
Synonym: Bexane, Can-Trol, Legumex, Thistrol, Thitrol, Trifolex, Tropotox
Chemical Name: 4-(4-chloro-2-methylphenoxy)butanoic acid; 4-(4-chloro-2-methylphenoxy)-butyric acid
Uses: herbicide for post-emergence control of annual and perennial broadleaf weeds in cereals, clovers, sainfoin, groundnuts, peas, etc. and also used to control broadleaf and woody weeds in forestry.
CAS Registry No: 94-81-5
Molecular Formula: C₁₁H₁₃ClO₃
Molecular Weight: 228.672
Melting Point (°C):
Boiling Point (°C):
> 280 (Tomlin 1994)
Density (g/cm³ at 22°C):
1.254 (Tomlin 1994)
Molar Volume (cm³/mol):
255.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
4.80 (potentiometric titration, Nelson & Faust 1969)
4.84 (Worthing & Hance 1991; Tomlin 1994)
Enthalpy of Fusion, ∆Hₜₙ (kJ/mol):
34.31 (DSC method, Plato 1972)
Entropy of Fusion, ∆Sₜₙ (J/mol K):
(Fugacity Ratio at 25°C (assuming ∆Sₜₙ = 56 J/mol K), F: 0.184 (mp at 100°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
41 (shake flask-UV, Leopold et al. 1960)
44 (rm. temp., Melnikov 1971)
44 (Bailey & White 1965; Martin & Worthing 1977; Hartley & Kidd 1987)
Vapor Pressure (Pa at 25°C or as indicated):
5.77 × 10⁻⁵, 9.83 × 10⁻⁵ (20, 25°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
3.22 × 10⁻⁴ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kᵥₖ:
4.60 (selected, Dao et al. 1983)
3.53 (RP-HPLC-k’ correlation, Braumann et al. 1983)
3.473 (countercurrent LC, Ilchmann et al. 1993)
2.79 (Tomlin 1994)
3.43 (selected, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.86 (calculated-S, Kenaga 1980)
Sorption Partition Coefficient, log Kₒₖ:
2.73 (soil, calculated-S, Kenaga 1980)
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:

- Soil: duration of residual activity in soil is ca. 3–4 months (Hartley & Kidd 1987; Tomlin 1994).
17.1.1.48 Mecoprop

![Chemical Structure of Mecoprop]

Common Name: Mecoprop
Synonym: Compitox, Duplosan, Hedonal, Iso-Cornox, Kilprop, MCPP, Mecopex, Mepro, Methoxone, Propal
Chemical Name: (±)-2-(4-chloro-2-methylphenoxy)propanoic acid; (±)-2-(4-chloro-o-tolyl-oxy)propionic acid
Uses: herbicide for post-emergence control of broadleaf weeds in wheat, barley, rye, herbage seed crops, grassland, and under fruit trees and vines, etc.
CAS Registry No: 7085-19-0
Molecular Formula: C_{10}H_{11}ClO_3
Molecular Weight: 214.645
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
233.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pH:
3.75 (Bailey & White 1965; quoted, Que Hee et al. 1981)
3.105 (Cessna & Grover 1978)
3.78 (Worthing & Hance 1991)
3.11 (Armbrust 2000)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
28.87 (DSC method, Plato 1972)
Enteropy 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):
895 (Martin 1961; Bailey & White 1965)
891 (Bailey & White 1965)
620 (Martin & Worthing 1977)
734 (Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
< 1.0 × 10⁻⁵ (20°C, Hartley & Kidd 1987)
3.10 × 10⁻⁴ (20°C, Worthing & Hance 1991)
0.0 (selected, Halfon et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
7.43 × 10⁻⁵ (calculated-P/C, this work)
1.11 × 10⁻⁵ (quoted lit., Armbrust 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
3.94 (selected, Dao et al. 1983)
2.83 (RP-HPLC-k’ correlation, Braumann et al. 1983)
0.10 (Worthing & Hance 1991)
0.09; 3.126 (quoted; countercurrent LC, Ilchmann et al. 1993)
3.13 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.20  (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{oc}:
2.11  (soil, calculated, Kenaga 1980, quoted, Bottini & Funari 1992)
1.30  (selected, Lohninger 1994)
1.30  (quoted lit., Armburst 2000)

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

Volatilization:
Photolysis: photodegradation t½ < 10 -15 d on 3 Spanish natural dry soils; t½ = 15–50 d on 10% peat-amended dry soils; degradation t½ ~ 2–5.5 d on moist soils at field capacity and saturated soils for degradation at 0.1 and 2 exposures days; and t½ = 13–32 d on moist soils at field capacity and saturated soils for degradation at 2.4 and 10 exposure days (Romero et al. 1998)

Oxidation: photooxidation t½ = 3.8–37.8 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable aqueous hydrolysis rate at pH 5, 7, pH 9; measured hydroxy radical rate constant for mecoprop k = 9.0 × 10^{12} M^{-1} h^{-1} (Armbrust 2000)

Biodegradation: aqueous aerobic t½ = 168–240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991); aqueous anaerobic t½ = 672–4320 h, based on anaerobic digest or sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991);

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:
Air: t½ = 3.8–37.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: t½ = 168–240 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Groundwater: t½ = 336–4320 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)
reported t½ = 8 d (Bottoni & Funari 1992).

Sediment:
Soil: t½ = 168–240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991);
reported t½ = 8 d (Bottoni & Funari 1992);
t½ = 21 d (selected, Halfon et al. 1996)
photodegradation t½ < 10 -15 d on 3 Spanish natural dry soils; t½ = 15–50 d on 10% peat-amended dry soils; degradation t½ ~ 2–5.5 d on moist soils at field capacity and saturated soils for degradation at 0.1 and 2 exposures days; and t½ = 13–32 d on moist soils at field capacity and saturated soils for degradation at 2.4 and 10 exposure days (Romero et al. 1998).

Biota:
17.1.1.49 Metolachlor

Common Name: Metolachlor
Synonym: Bicep, CGA 24705, Codal, Cortoran multi, Dual, Metetilachlor, Milocep, Ontrack 8E, Pennant, Primagram, Primextra
Chemical Name: 2-chloro-6'-ethyl-N-(2-methoxy-1-methylethyl)acet-o-toluidide; 2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide
Uses: pre-emergence herbicide to control most annual grasses and weeds in beans, chickpeas, corn, cotton, milo, okra, peanuts, peas, potatoes, sunflower, soybeans and some ornamentals.
CAS Registry No: 51218-45-2
Molecular Formula: C_{15}H_{22}ClNO_{2}
Molecular Weight: 283.795
Melting Point (°C): liquid
Boiling Point (°C):
- 100 (at 0.001 mmHg, Herbicide Handbook 1989; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Density (g/cm³ at 20°C):
- 1.12 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
- 1.085 (Herbicide Handbook 1989)
Molar Volume (cm³/mol):
- 340.0 (calculated-Le Bas method at normal boiling point)
- 258.0 (calculated-density)
Dissociation Constant pKₐ:
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/mL or mg/L at 25°C or as indicated):
- 530 (Martin & Worthing 1977)
- 440 (selected, Ellgehausen et al. 1980)
- 520 (20°C, Ashton & Crafts 1981; Spencer 1982)
- 530 (shake flask-HPLC, Ellgehausen et al. 1981)
- 530 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)
- 488 (Tomlin 1994)
- 530 (20–25°C, selected, Hornsby et al. 1996)
- 531, 505 (supercooled liquid S₂; literature derived value LDV, final adjust value FAV, Muir et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.00170 (20°C, Hartley & Graham-Bryce 1980)
- 0.00173 (20°C, Ashton & Crafts 1981)
- 0.00173 (20°C, volatilization rate, Burkhard & Guth 1981)
- 0.00170 (20°C, Hartley & Kidd 1987)
- 0.00170 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)
- 0.00173 (20°C, Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)
- 4.20 × 10⁻³, 6.60 × 10⁻², 0.70, 5.40, 33.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
\[ \log \left( \frac{P}{Pa} \right) = 13.115 - 4619.7/(T/K); \text{measured range 32.5–140°C} \] (gas saturation-GC, Rordorf 1989)
- 0.00420 (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.00092 (Hartley & Graham-Bryce 1980)
0.00093 (20°C, volatilization rate, Burkhard & Guth 1981)
0.00091 (20°C, calculated-P/C as per Worthing & Walker 1987)
0.00093 (20°C, calculated-P/C, Montgomery 1993)
0.00082 (20°C, calculated-P/C, Majewski & Capel 1995)
0.00244 (calculated-P/C, Otto et al. 1997)
0.00782 (20°C, distilled water, wetted wall column-GC, Rice et al. 1997b)
0.00110 (calculated-P/C, this work)
0.00238* (20°C, gas stripping-GC/MS, measured range 283.05–299.45 K, Feigenbrugel et al. 2004)

\[ H'/(M\text{ atm}^{-1}) = (3.0 \pm 0.4) \times 10^{-11} \exp[(10200 \pm 1000)/(T/K)]; \text{ temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)} \]

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

3.13 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)
3.28 (shake flask-HPLC, Ellgehausen et al. 1981)
3.45 (Worthing & Hance 1991)
2.93, 3.45 (Montgomery 1993)
3.13, 3.28 (quoted, Sangster et al. 1993)
2.90 (Tomlin 1994)
3.45 (Milne 1995)
3.31, 2.95 (selected, calculated-f const., Pinsuwan et al. 1995)
3.13 (recommended, Hanch et al. 1995)
2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
3.10 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:

9.37 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:

1.813 (log BF-bioaccumulation of algae, Ellgehausen et al. 1980)
0.733 (log BF-bioaccumulation of daphnids, Ellgehausen et al. 1980; quoted, Geyer et al. 1991)
0.851 (log BF-bioaccumulation of catfish, Ellgehausen et al. 1980)
1.26 (calculated-S, Kenaga 1980)
1.15 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

2.15 (soil, calculated-S, Kenaga 1980)
2.26 (soil, screening model calculations, Jury et al. 1987b)
2.00, 2.15, 2.28, 2.30 (soil, quoted values, Bottini & Funari 1992)
2.46, 2.46 (soil, quoted explt., calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)
2.08–2.49 (Montgomery 1993; Tomlin 1994)
2.46 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)
2.43 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.28, 2.19, 2.69 (soils: organic carbon OC \( \geq 0.1\% \), OC \( \geq 0.5\% \), 0.1 \( \leq \) OC < 0.5%, average, Delle Site 2001)

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

Volatilization:
Herbicides

Photolysis: under optimum exposure conditions to natural sunlight, $t_{1/2} \approx 8$ d (Herbicide Handbook 1989).
Oxidation: $k_{\text{OH}} = 5.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in gas phase with atmospheric lifetime of 0.9 h but reduced to 0.4 h at 283 K; $\log k_{\text{OH(aq.)}} = 1.2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ in aqueous phase (Feigenbrugel et al. 2004).
Hydrolysis: $t_{1/2} > 200$ d at 20°C and $1 \leq \text{pH} \leq 9$ (Montgomery 1993); $t_{1/2} > 200$ d ($2 \leq \text{pH} \leq 10$) (Tomlin 1994).
Biodegradation: overall degradation rate constant $k = 0.0154 \text{ h}^{-1}$ with $t_{1/2} = 45.0$ h in sewage sludge and rate constant $k = 0.0460 \text{ d}^{-1}$ with $t_{1/2} = 15.1$ d in garden soil (Müller & Buser 1995).

Biotransformation:

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

- $k_2 = 9.11 \text{ d}^{-1}$ (catfish, Ellgehausen et al. 1980)
- $k_1 = 0.336 \text{ h}^{-1}$, $k_2 = 0.024 \text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported $t_{1/2} = 20, 30, 42,$ and $47–107$ d (Bottoni & Funari 1992)

- degradation time 500–1000 d (Tomlin 1994).

Sediment:

Soil: $t_{1/2} = 15–38$ d in clay loam soils and $t_{1/2} = 33–100$ d in sandy loam soils (Zimdahl & Clark 1982; quoted, Montgomery 1993);

- $t_{1/2} = 42$ d from field $t_{1/2} = 3–4$ wk by using lysimeters (Bowman 1990);
- $t_{1/2} = 80, 99$ and 142 d for the disappearance from upper 15 cm on an Ontario clay loam soil while the decline was followed for 332, 364 and 370 d, respectively, in 1987, 1988 and 1989 (Frank et al. 1991);
- $t_{1/2} \approx 6$ d in soil (Worthing & Hance 1991; quoted, Montgomery 1993);

- reported $t_{1/2} = 20, 30, 42, 47–107$ d (Bottoni & Funari 1992)

- field $t_{1/2} = 90$ d at 20–25°C (selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Halfon et al. 1996; Hornsby et al. 1996);

- soil $t_{1/2} = 40$ d (Pait et al. 1992);

- soil $t_{1/2} = 28–46$ d (Di Guardo et al. 1994);

- $t_{1/2} \approx 30$ d (Tomlin 1994);

- degradation $t_{1/2} = 15.1$ d in garden soil (Müller & Buser 1995);

- $t_{1/2} \approx 28.3$ d under conventional tillage, $t_{1/2} \approx 25.61$ d under ridge tillage and $t_{1/2} \approx 8.63$ d with no tillage (Otto et al. 1997).

Biota: $t_{1/2} = 1.15$ d in catfish (Ellgehausen et al. 1980);

- biochemical $t_{1/2} = 42$ d from screening model calculations (Jury et al. 1987b).

### TABLE 17.1.1.49.1

Reported Henry’s law constants of metolachlor at various temperatures

<table>
<thead>
<tr>
<th>$t/\degree\text{C}$</th>
<th>gas stripping-GC/MS</th>
<th>$t/\degree\text{C}$</th>
<th>gas stripping-GC/MS</th>
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<tbody>
<tr>
<td>283.05</td>
<td>$5.39 \times 10^{-4}$</td>
<td>293.25</td>
<td>$2.262 \times 10^{-3}$</td>
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<tr>
<td>283.15</td>
<td>$6.34 \times 10^{-4}$</td>
<td>297.55</td>
<td>$3.099 \times 10^{-3}$</td>
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<tr>
<td>283.25</td>
<td>$8.126 \times 10^{-4}$</td>
<td>298.05</td>
<td>$4.053 \times 10^{-3}$</td>
</tr>
<tr>
<td>283.65</td>
<td>$8.465 \times 10^{-4}$</td>
<td>298.15</td>
<td>$4.757 \times 10^{-3}$</td>
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<td>285.55</td>
<td>$8.01 \times 10^{-4}$</td>
<td>298.15</td>
<td>$4.312 \times 10^{-3}$</td>
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<td>287.55</td>
<td>$1.088 \times 10^{-3}$</td>
<td>299.45</td>
<td>$4.170 \times 10^{-3}$</td>
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<td>289.45</td>
<td>$1.193 \times 10^{-3}$</td>
<td>291.55</td>
<td>$1.419 \times 10^{-3}$</td>
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<td>291.55</td>
<td>$\ln H' = A - B/(T/K)$</td>
<td>293.05</td>
<td>$2.702 \times 10^{-3}$</td>
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<td>293.05</td>
<td>$2.471 \times 10^{-3}$</td>
<td>24.2298</td>
<td>$-24.2298$</td>
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<td>293.15</td>
<td>$2.282 \times 10^{-3}$</td>
<td>B</td>
<td>10200</td>
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<tr>
<td>293.15</td>
<td>$2.227 \times 10^{-3}$</td>
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FIGURE 17.1.149.1 Logarithm of Henry’s law constant versus reciprocal temperature for metolachlor.
### 17.1.1.50 Metribuzin

![Chemical structure of Metribuzin](image)

**Common Name:** Metribuzin  
**Synonym:** Metribuzine, Lexone, Preview, Sencor, Sencoral, Sencorer, Sencorex  
**Chemical Name:** 4-amino-6-(t-butyl)-3-(methylthio)-1,2,4-triazin-5-(4H)-one  
**CAS Registry No:** 21087-64-9  
**Uses:** herbicide  
**Molecular Formula:** C₈H₁₄N₄OS  
**Molecular Weight:** 214.288  

<table>
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<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>126</td>
<td>(Lide 2003)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>132.2 Pa</td>
<td>(Tomlin 1994)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>1.31</td>
<td>(Hartley &amp; Kidd 1987; Montgomery 1993; Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>1.28</td>
<td>(Herbicide Handbook 1989)</td>
</tr>
<tr>
<td>Dissociation Constant pKᵦ</td>
<td>13.0</td>
<td>(Wauchope et al. 1992; Hornsby et al. 1996)</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>(pKᵦ, Montgomery 1993)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ∆Hᵦ</td>
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<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ∆Sᵦ</td>
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<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C</td>
<td>F: 0.102 (mp at 126°C)</td>
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</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1220</td>
<td>(Kenaga &amp; Goring 1980; Kenaga 1980b; Verschueren 1983)</td>
</tr>
<tr>
<td></td>
<td>1220</td>
<td>(Herbicide Handbook 1989)</td>
</tr>
<tr>
<td></td>
<td>1050</td>
<td>(20°C, Montgomery 1993; Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>1065</td>
<td>(20–25°C, reported as 4.97E + 01 mol/m³, Majewski &amp; Capel 1995)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C or as indicated):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>&lt; 1.3 × 10⁻³; 2.67 × 10⁻² (20°C; 60°C, Herbicide Handbook 1989)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.8 × 10⁻⁵ (20°C, Montgomery 1993)</td>
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</tr>
<tr>
<td></td>
<td>5.89 × 10⁻⁴ (20–25°C, Majewski &amp; Capel 1995)</td>
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</tr>
<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C):</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>&lt; 1.3 × 10⁻³ (Spencer 1982; Worthing 1987; Hartley &amp; Kidd 1987)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.21 × 10⁻⁵ (calculated-P/C, Montgomery 1993)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.18 × 10⁻⁵ (calculated-P/C, Majewski &amp; Capel 1995)</td>
<td></td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log Kₐ₀w:</td>
<td></td>
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<tr>
<td></td>
<td>1.60, 1.70 (quoted, Montgomery 1993)</td>
<td></td>
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<tr>
<td></td>
<td>1.58</td>
<td>(pH 5.6, Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>1.70</td>
<td>(LOGPSTAR or CLOGP data, Sabljic et al. 1995)</td>
</tr>
</tbody>
</table>
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:
- 2.46, 1.48, < 1.30 (algae, activated sludge, fish in 3-d testing, Korte et al. 1978)
- 1.77, 1.75 (Chlorella, calculated-solubility, Geyer et al. 1981)
- 1.77, 1.48, 1.04 (algae, activated sludge, Golden orfe, Geyer et al. 1982)
- 1.04, 0.602 (calculated-solubility, calculated-$K_{OW}$, Kenaga 1980a)
- 1.48, 1.78, 1.0 (activated sludge, algae, Golden ide, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:
- 1.98 (soil, Kenaga & Goring 1980)
- 1.98; 1.94 (quoted, calculated-$K_{OW}$, Kenaga 1980b)
- 0.954–2.72 (soil, literature range, Wauchope et al. 1992)
- 1.80 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.94–1.98, 2.18 (soil, Bottoni & Funari 1992)
- 1.80–2.72 (soil, Montgomery 1993)
- 1.78 (soil, Senseman et al. 1997)
- 1.71 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.71; 1.68, 1.33 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.05, 2.06, 2.04 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, 0.1 $\leq OC < 0.5\%$, average, Delle Site 2001)

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

Volatilization:
- Photolysis: photodecomposition in water is very rapid with $t_{1/2} < 1$ d; on soil surface under natural sunlight conditions, $t_{1/2} = 14–25$ d (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2}$ ~ 1 wk in pond water (Hartley & Kidd 1987; Montgomery 1993).

Biodegradation: undergoes microbial degradation in moist soil (Worthing 1987)

Biotransformation:

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

Half-Lives in the Environment:

Air:
- Surface water: hydrolysis $t_{1/2}$ ~ 1 wk in pond water (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);
- stable to dilute acids and alkalis, $t_{1/2} = 6.7$ h at pH 1.2 and 37°C; $t_{1/2} = 569$ h at pH 4, $t_{1/2} = 47$ d at pH 7 and $t_{1/2} = 191$ h at pH 9 for 70°C (Tomlin 1994).

Ground water: reported half-life or persistence $t_{1/2} = 4–25$, 17–301 and 56 d (Bottoni & Funari 1992).

Sediment:
- Soil: undergoes microbial degradation in moist soil (Worthing 1983, 1987);
- half-life varies with soil types, $t_{1/2} = 90–115$ d for Red River, Almasippi, and Stockton soils the 3 times this period for Newdale soil for normal application rates (Verschueren 1983);
- $t_{1/2} = 1–2$ months in soil (Hartley & Kidd 1987; Tomlin 1994);
- $t_{1/2} = 30–60$ d in various soil types varies greatly with climatic conditions, during the growing season (Herbicide Handbook 1989);
- $t_{1/2} = 9–12$ d irrespective of the number of previous treatments in the field; $t_{1/2} = 25–40$ d irrespective of the pretreatment history of the soil at 20°C in the laboratory (Walker & Welch 1992) reported $t_{1/2} = 23–120$ d and the recommended field $t_{1/2} = 40$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997);
- half-lives of in two surface soil microcosms under nitrate, $t_{1/2} = 157$ d and non-nitrate, $t_{1/2} = 187$ and 349 d in reducing culture conditions at 16.4°C (Pavel et al. 1999).

Biota: in mammals, following oral administration, 90% elimination within 96 h (Hartley & Kidd 1987).
17.1.1.51 Molinate

Common Name: Molinate
Synonym: Felan, Higalnate, Hydram, Jalan, Molmate, Ordram, Stauffer R 4572, Sakkimok, Yalan, Yulan
Chemical Name: 1H-azepine-1-carbothioic acid, hexahydro, S-ethyl ester; ethyl 1-hexa-methyleneiminecarbothioate
Uses: selective herbicide to control the germination of annual grasses and broadleaf weeds in rice crops.
CAS Registry No: 2212-67-1
Molecular Formula: C₉H₁₇NOS
Molecular Weight: 187.302
Melting Point (°C): < 25 (Montgomery 1993)
Boiling Point (°C):
  202 (at 10 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)
  117 (at 10 mmHg, Montgomery 1993)
Density (g/cm³ at 20°C):
  1.064 (Hartley & Kidd 1987)
  1.0643 (Herbicide Handbook 1989; Montgomery 1993)
  1.063 (Worthing & Hance 1991; Milne 1995)
Molar Volume (cm³/mol):
  220.6 (calculated-Le Bas method at normal boiling point)
  176.1 (calculated-density)
Dissociation Constant pKₐ
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):
  800 (Martin & Worthing 1977)
  800–912 (Weber et al. 1980)
  912 (21°C, Spencer 1982)
  870 (Kanazawa 1989)
  880 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
  0.748 (20°C, Weber 1972; Worthing & Walker 1987)
  0.746 (20°C, Khan 1980)
  0.185 (20°C, GC-RT correlation, Kim 1985)
  0.413 (Seiber et al. 1986, 1989)
  0.746 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
  0.746 (Herbicide Handbook 1989; Worthing & Hance 1991)
  0.746 (20–25°C, selected, Wauchope et al. 1992)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  0.097 (calculated-P/C, Seiber et al. 1986, 1989)
  0.314 (20°C, calculated-P/C, Suntio et al. 1988)
  0.159 (20°C, calculated-P/C as per Worthing & Walker 1987;)
  0.159 (20°C, calculated-P/C, Muir 1991)
Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.21 (shake flask-GC, Kanazawa 1981)
2.88 (Worthing & Hance 1991; Tomlin 1994)
2.88 (Montgomery 1993)
3.13 (RP-HPLC-RT correlation, Saito et al. 1993)
3.26 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.21 (recommended, Sangster 1993)
2.88 (Milne 1995)
3.21 (recommended, Hansch et al. 1995)
3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log BCF$:

1.15 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.41 ($Pseudorasbora parva$, Kanazawa 1981)

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

2.04 (soil, calculated-S, Kenaga 1980)
1.92 (average of 2 soils, Kanazawa 1989)
1.92, 2.04 (soil, quoted values, Bottoni & Funari 1992)
1.92, 2.46 (soil, quoted exptl., calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
1.93–1.97 (Montgomery 1993)
2.28 (selected, Lohninger 1994)
1.92 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.07 (soil, quoted lit., Armbrust 2000)
1.92; 2.31, 1.86 (soil, quoted exptl.; estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatile: $k = 0.0150 \text{ h}^{-1}$ (average of 2 runs, Seiber et al. 1986); 1.1 kg ha$^{-1}$ (1st 4 day) from flooded rice fields (Seiber et al. 1986; Seiber & McChesney 1987); estimated $t_{1/2} = 43 \text{ d}$ from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2} = 7–10 \text{ d}$ for 8–10 µg mL$^{-1}$ to degrade in distilled water under > 290 nm light (Soderquist et al. 1977; quoted, Cessna & Muir 1991);

$\text{OH}$ reaction: $t_{1/2} = 96 \text{ h}$ for < 5% of 0.2 µg mL$^{-1}$ to degrade in distilled water under sunlight (Deuel et al. 1978; quoted, Cessna & Muir 1991);

$\text{O}_{3}$ reaction: $t_{1/2} = 245 \text{ h}$ for 2–54% of 10 µg mL$^{-1}$ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991).

Oxidation: calculated life-time of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992);

measured rate constant for reaction with hydroxyl radical, $k(\text{aq.}) = 0.85 \times 10^9 \text{ M}^{-1}\cdot\text{s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996);

measured hydroxy radical reaction rate constant for molinate $k = 7.7 \times 10^{12} \text{ M}^{-1}\cdot\text{h}^{-1}$ (Armbrust 2000).

Hydrolysis: $t_{1/2} > 10 \text{ d}$ in aqueous buffer at pH 5–9 in the dark (Soderquist et al. 1977; quoted, Muir 1991); stable aqueous hydrolysis rate at pH 5, 7, 9 (Armbrust 2000).
Biodegradation: \( t_{1/2} \approx 16 \text{ d} \) for 0.2 \( \mu \text{g mL}^{-1} \) to biodegrade in flooded soils (Deuel et al. 1978; quoted, Muir 1991); 
\( t_{1/2} = 10 \text{ wk} \) for 4.2 \( \mu \text{g mL}^{-1} \) to biodegrade in flooded soil and \( t_{1/2} < 2 \text{ wk} \) in water both at 21–26°C (Thomas & Holt 1980; quoted, Muir 1991); 
aerobic rate constant, \( k = 2.22 \times 10^{-3} \text{ h}^{-1} \) (Armbrust 2000).

Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Surface water: \( t_{1/2} = 84 \text{ h} \) from dissipation from flooded rice fields (Seiber & McChesney 1987; quoted, Seiber et al. 1989).
Ground water: reported half-lives or persistence, \( t_{1/2} = 3–14, 8–25 \) and 40–160 d (Bottoni & Funari 1992)
Sediment:
Soil: persistence of 2 months in soil (Wauchope 1978); 
\( t_{1/2} \approx 3 \text{ wk} \) in moist loam soils at 21–27°C (Herbicide Handbook 1989); 
selected field \( t_{1/2} = 21 \text{ d} \) (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996); 
soil \( t_{1/2} = 21 \text{ d} \) (Pait et al. 1992); 
reported \( t_{1/2} = 3–14 \text{ d}, 8–25 \) d and 40–160 d (Bottoni & Funari 1992).
Biota:
17.1.1.52 Monolinuron

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\begin{center}
\includegraphics[width=0.5\textwidth]{monolinuron.png}
\end{center}
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Common Name: Monolinuron  
Synonym: Afesin, Aresin, Arresin, Hoe 02747  
Chemical Name: 3-(4-chlorophenyl)-1-methoxy-1-methylurea; \(N^\prime\)-(4-chlorophenyl)-\(N\)-methoxy-\(N\)-methylurea  
Uses: herbicide for pre- or post-emergence control of annual broadleaf weeds and annual grasses in asparagus, berry fruit, cereals, maize, field beans, vines, leeks, onions, potatoes, herbs, lucerne, flowers, ornamental shrubs and trees, etc.  
CAS Registry No: 1746-81-2  
Molecular Formula: \(\text{C}_9\text{H}_11\text{ClN}_2\text{O}_2\)  
Molecular Weight: 214.648  
Melting Point (°C):  
\hspace{1cm}77 \hspace{1cm} (Lide 2003)  
Boiling Point (°C):  
Density (g/cm³ at 20°C):  
Molar Volume (cm³/mol):  
\hspace{1cm}224.0 \hspace{1cm} (calculated-Le Bas method at normal boiling point)  
Dissociation Constant \(pK_a\):  
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), \(F\): 0.309 (mp at 77°C)  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
\hspace{1cm}735 \hspace{1cm} (20°C, Melnikov 1971)  
\hspace{1cm}735 \hspace{1cm} (Spencer 1973, 1982)  
\hspace{1cm}580 \hspace{1cm} (Martin & Worthing 1977; Khan 1980)  
\hspace{1cm}735 \hspace{1cm} (Worthing & Walker 1983, 1987, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
\hspace{1cm}735 \hspace{1cm} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
Vapor Pressure (Pa at 25°C or as indicated):  
\hspace{1cm}0.02 \hspace{1cm} (22°C, Khan 1980; Hartley & Kidd 1987)  
\hspace{1cm}0.0015 \hspace{1cm} (20°C, Spencer 1982)  
\hspace{1cm}6.40 \hspace{1cm} (65°C, Worthing & Hance 1991)  
\hspace{1cm}0.02 \hspace{1cm} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
\hspace{1cm}0.0013, 0.10 \hspace{1cm} (20°C, 50°C, Tomlin 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
\hspace{1cm}0.0058 \hspace{1cm} (calculated-P/C, this work)  
Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):  
\hspace{1cm}1.60 \hspace{1cm} (Briggs 1969)  
\hspace{1cm}2.30 \hspace{1cm} (shake flask-UV, Briggs 1981)  
\hspace{1cm}1.60 \hspace{1cm} (selected, Dao et al. 1983)  
\hspace{1cm}1.99 \hspace{1cm} (RP-HPLC-k’ correlation, Braumann et al. 1983)  
\hspace{1cm}2.22 \hspace{1cm} (shake flask, Mitsutake et al.1986)  
\hspace{1cm}2.20 \hspace{1cm} (Worthing & Hance 1991; Tomlin 1994)  
\hspace{1cm}2.16 \hspace{1cm} (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)  
\hspace{1cm}2.30 \hspace{1cm} (recommended, Sangster 1993)  
\hspace{1cm}2.30 \hspace{1cm} (recommended, Hansch et al. 1995)  
\hspace{1cm}2.31 \hspace{1cm} (Pomona-database, Müller & Kördel 1996)
Herbicides

2.16 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.23; 1.00 (calculated-S, calculated-$K_{OC}$, Kenaga 1980)
1.85 (activated sludge, Freitag et al. 1982, 1984, 1985)
1.52, < 1.0 (algae, golden orfe, Freitag et al. 1982)
1.60, 1.30 (algae, golden ide, Freitag et al. 1985)

Sorption Partition Coefficient, log $K_{OC}$:
2.30 (soil, Hamaker & Thompson 1972)
2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.60 (reported as log $K_{OM}$, Briggs 1981)
2.36, 2.08, 1.21 (estimated-S, calculated-S and mp, calculated-$K_{OM}$, Karickhoff 1981)
2.40–2.70 (soil, Worthing & Hance 1991)
2.26–2.30, 2.40–2.70 (soil, quoted values, Bottoni & Funari 1992)
1.78 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.10 (soil, calculated-MCI `χ, Sabljic et al. 1995)
1.78; 2.33 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.44, 1.50, 1.71, 1.754, 2.45 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.05, 1.72, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.10; 2.04, 2.31 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.88, 1.88 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Photolysis: $t_{1/2} = 23$ h for 66% of 286 µg/mL to degrade in distilled water under > 300 nm light (Kotzias et al. 1974; quoted, Cessna & Muir 1991).

Half-Lives in the Environment:
Air:
Surface water:
Ground water: reported half-lives or persistence, $t_{1/2} = 45–60$ d (Bottoni & Funari 1992)
Sediment:
Soil: reported $t_{1/2} = 45–60$ d (Worthing & Hance 1991);
estimated field $t_{1/2} = 60$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:
17.1.1.53 Monuron

Common Name: Monuron

Synonym: Chlorfenidim, CMU, Karmex, Lirobetarex, Monurex, Monurox, Rosuran, Telvar, Urox

Chemical Name: \( \text{N}^\prime-(4\text{-chlorophenyl})\text{-N-N-dimethylurea; 1,1-dimethyl-3-(p-chlorophenyl)urea} \)

Uses: herbicide; also as sugar cane flowering suppressant.

CAS Registry No: 150-68-5

Molecular Formula: \( \text{C}_9\text{H}_{11}\text{ClN}_2\text{O} \)

Molecular Weight: 198.648

Melting Point (°C):
- 170.5 (Kühne et al. 1995; Lide 2003)

Boiling Point (°C):
- 185–200 (decomposes, Montgomery 1993)

Density (g/cm\(^3\) at 20°C):
- 1.27 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm\(^3\)/mol):
- 202.9 (calculated-Le Bas method at normal boiling point)
- 173.0 (modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant \( pK_a \):

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), \( F: 0.0374 \) (mp at 170.5°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
- 203 (Freed 1966)
- 230 (Günther et al. 1968; Sanborn et al. 1977; Khan 1980; Ashton & Crafts 1981)
- 262 (shake flask-UV, Hurle & Freed 1972)
- 230 (Martin & Worthing 1977; Hartley & Kidd 1987)
- 200 (shake flask-HPLC, Ellgehausen et al. 1981)
- 200 (20°C, selected, Suntio et al. 1988)
- 275 (Spurlock 1992; Spurlock & Biggar 1994b)
- 230 (at pH 6.26, Montgomery 1993)

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):
- \( 7.60 \times 10^{-5}, 1.2 \times 10^{-5} \) (25, 27°C, Nex & Swezey 1954)
- \( 6.67 \times 10^{-5} \) (Bailey & White 1965)
- \( 6.72 \times 10^{-5} \) (20°C, Weber 1972; Worthing & Walker 1987)
- \( 5.33 \times 10^{-5} \) (30.35°C, Knudsen effusion, measured range 303.5–379.1 K, Wiedemann 1972)
- \( \log (P/\text{mmHg}) = 13.3052 - 5988.39/(T/K); \) temp range 303.5–379.1 K (Antoine eq., effusion, Wiedemann 1972)
- \( 6.70 \times 10^{-5} \) (OECD 1981)
- \( 2.30 \times 10^{-5} \) (calculated, Jury et al. 1983)
- \( 6.00 \times 10^{-5} \) (Hartley & Kidd 1987)
- \( 6.67 \times 10^{-5} \) (Budavari 1989)
- \( 2.30 \times 10^{-5} \) (selected, Taylor & Spencer 1990)
- \( 6.00 \times 10^{-5} \) (20°C, Montgomery 1993)
- \( 6.67 \times 10^{-5} \) (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

- 5.80 × 10⁻⁵ (20°C, volatilization rate, Burkhard & Guth 1981)
- 1.88 × 10⁻⁵ (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
- 3.00 × 10⁻³ (20°C, calculated-P/C, Suntio et al. 1988)
- 1.91 × 10⁻⁵ (calculated-P/C, Taylor & Glotfelty 1988)
- 5.60 × 10⁻⁵ (20°C, calculated-P/C, Muir 1991)
- 3.00 × 10⁻³ (20°C, calculated-P/C, Montgomery 1993)
- 6.60 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log Kₐₙₜ:

- 1.46, 1.66 (Briggs 1969)
- 1.80 (calculated-fragment const., Rekker 1977)
- 2.08 (shake flask-UV, Erkell & Walum 1979)
- 2.12 (Rao & Davidson 1980)
- 1.98 (shake flask-UV, Briggs 1981)
- 2.08 (shake flask, Ellgehausen et al. 1980)
- 1.66 (shake flask, Ellgehausen et al. 1981)
- 1.86 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 1.91 (RP-HPLC-k’ correlation Braumann et al. 1983)
- 1.80 (selected, Suntio et al. 1988)
- 2.12 (shake flask-HPLC, Spurlock 1992; Spurlock & Biggar 1994b)
- 1.46, 2.12 (Montgomery 1993)
- 1.86 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 1.94 (recommended, Sangster 1993)
- 1.89; 1.88 (shake flask-UV; RP-HPLC-k’ correlation, Liu & Qian 1995)
- 1.94 (recommended, Hansch et al. 1995)
- 1.99 (Pomona-database, Müller & Kördel 1996)
- 1.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.786 (log BF bioaccumulation factor for algae, Ellgehausen et al. 1980)
- 0.32 (log BF bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 0.245 (log BF bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 1.46 (calculated-S, Kenaga 1980)
- 0.699 (calculated-KOC, Kenaga 1980)
- 0.0 (TrieneAdes tardus, Belluck & Felsot 1981)
- 1.58, 1.67 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, log KOC:

- 2.00 (soil, Hamaker & Thompson 1972)
- 2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (av. of 18 soils, Rao & Davidson 1980)
- 1.70 (soil, converted from reported KOC, multiplied by 1,724, Briggs 1981)
- 2.58, 1.51 (estimated-S, calculated-S and mp, Karickhoff 1981)
- 1.07, 1.73, 2.58 (estimated-KOW, Karickhoff 1981)
- 2.03, 1.85; 2.17, 1.52 (estimated-KOW; solubilities, Madhun et al. 1986)
- 1.99; 2.12 (quoted; calculated-MCI, Gerstl & Helling 1987)
- 2.26 (screening model calculations, Jury et al. 1987a,b; Jury & Ghoodrati 1989)
- 1.99, 2.33 (Montgomery 1993)
- 1.99 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 2.29 (calculated-KOW, Liu & Qian 1995)
- 1.95 (soil, calculated-MCI, Sabljic et al. 1995)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis: $t_{1/2} = 14$ d for 6% of 200 µg mL$^{-1}$ to degrade in distilled water under sunlight (Crosby & Tang 1969; quoted, Cessna & Muir 1991);

$\text{HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996}$


1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

1.80, 1.80 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Photolysis: $t_{1/2} = 14$ d for 6% of 200 µg mL$^{-1}$ to degrade in distilled water under sunlight (Crosby & Tang 1969; quoted, Cessna & Muir 1991);

$\text{HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996}$


1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

1.80, 1.80 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Oxidation:

Hydrolysis: $t_{1/2} > 4$ months for 3974 µg mL$^{-1}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: aerobic $t_{1/2} \sim 7$ d for 0.01 µg mL$^{-1}$ to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);

$\text{HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996}$


1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

1.80, 1.80 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Oxidation:

Hydrolysis: $t_{1/2} > 4$ months for 3974 µg mL$^{-1}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: aerobic $t_{1/2} \sim 7$ d for 0.01 µg mL$^{-1}$ to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);

$\text{HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996}$


1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

1.80, 1.80 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Biotransformation:

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

$\text{k}_2 = 21.05$ d$^{-1}$ (catfish, Ellgehausen et al. 1980)

Half-Lives in the Environment:

Air:

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971).

Ground water:

Sediment:

Soil: $t_{1/2} = 5.0$ months at 15°C and 4.1 months at 30°C in soils (Freed & Haque 1973);

reported $t_{1/2} = 166$ d from screening model calculations (Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989);

$\text{HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996}$


1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

1.80, 1.80 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Biota: $t_{1/2} = 0.45$ d in catfish (Ellgehausen et al. 1980);

biochemical $t_{1/2} = 166$ d from screening model calculations (Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989).
### TABLE 17.1.53.1
Reported vapor pressures of monuron 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>303.5</td>
<td>5.33 × 10⁻⁵</td>
<td>358.7</td>
<td>0.0536</td>
</tr>
<tr>
<td>316.0</td>
<td>2.44 × 10⁻⁴</td>
<td>360.2</td>
<td>0.0561</td>
</tr>
<tr>
<td>329.8</td>
<td>2.16 × 10⁻³</td>
<td>379.1</td>
<td>0.399</td>
</tr>
<tr>
<td>330.6</td>
<td>1.53 × 10⁻³</td>
<td></td>
<td></td>
</tr>
<tr>
<td>330.6</td>
<td>2.22 × 10⁻³</td>
<td>338.8</td>
<td>7.05 × 10⁻³</td>
</tr>
<tr>
<td>341.4</td>
<td>9.45 × 10⁻³</td>
<td></td>
<td></td>
</tr>
<tr>
<td>345.7</td>
<td>0.0105</td>
<td></td>
<td></td>
</tr>
<tr>
<td>349.5</td>
<td>0.0204</td>
<td></td>
<td></td>
</tr>
<tr>
<td>357.0</td>
<td>0.0529</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 114.6$$

### FIGURE 17.1.53.1
Logarithm of vapor pressure versus reciprocal temperature for monuron.
17.1.1.54 Napropamide

![Chemical Structure of Napropamide](image)

Common Name: Napropamide

Synonym: Devrinol

Chemical Name: 2-(α-naphthloxy)-N,N-diethylpropionamide

CAS Registry No: 15299-99-7

Uses: herbicide

Molecular Formula: C₁₇H₂₁NO₂

Molecular Weight: 271.355

Melting Point (°C):

75 (Worthing & Walker 1987; Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

Dissociation Constant pKₐ:

2.93 (Woodburn et al. 1993)

Enthalpy of Fusion, ΔHₕₜₜ (kJ/mol):

Entropy of Fusion, ΔSₕₜₜ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔSₕₜₜ = 56 J/mol K), F: 0.323 (mp at 75°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

69 (shake flask-LSC or GC, Gerstl & Mingelgrin 1984)


Vapor Pressure (Pa at 25°C or as indicated):

2.67 × 10⁻⁴ (Spencer 1982)

5.3 × 10⁻⁴ (Herbicide Handbook 1989)

5.3 × 10⁻⁴ (Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)


Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

0.00294 (calculated-P/C, Montgomery 1993)

0.00197 (20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K₁₀₆W:

3.08 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

3.6 (Montgomery 1993)

3.30 (Tomlin 1994)

3.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K₁₀₆ₐ:

Bioconcentration Factor, log BCF or log Kᵦ:

Sorption Partition Coefficient, log Kₒₑ:

2.04–3.09 (various soils, Mingelgrin & Gestl 1983)

2.82, 3.56 (soil: quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.62  (soil, average of log K_{OC} values, Gerstl 1990)  
3.52–4.29; 3.72 at pH 2, 3.35 at pH 6 (Dead sea sediment, Gestl & Kilger 1990)  
2.62–3.54; 3.54 at pH 2, 3.40 at pH 6 (Kinnert F sediment, Gestl & Kilger 1990)  
2.71–3.62; 3.62 at pH 2, 3.27 at pH 6 (Kinnert G sediment, Gestl & Kilger 1990)  
2.40–3.31; 3.31 at pH 2, 3.20 at pH 5 (Oxford soil, Gestl & Kilger 1990)  
2.39–3.15; 3.15 at pH 2, 2.88 at pH 6 (Malkiya soil, Gestl & Kilger 1990)  
2.28–3.29; 3.29 at pH 2, 3.09 at pH 5 (Neve Ya’ar soil, Gestl & Kilger 1990)  
2.85  (soil, Wauchope et al. 1992; Hornsby et al. 1996)  
2.29–3.99  (soil/sediment, literature range, Montgomery 1993)  
2.83  (soil, Montgomery 1993)  
2.62  (soil, calculated-MCI \chi, Sabljic et al. 1995)  
2.58, 2.58, 2.61  (soils: organic carbon OC \geq 0.1\%, OC \geq 0.5\%, 0.1 \leq OC < 0.5\%, average, Delle Site 2001)  
2.80  (sediment: organic carbon OC \geq 0.5\%, average, Delle Site 2001)  

Environmental Fate Rate Constants, k, or Half-Lives, \( t_{\frac{1}{2}} \):  
Volatilization: very little loss occurred by volatilization from soil surface (Herbicide Handbook 1989).  
Photolysis: under condition of high sunlight intensity in the summer, \( t_{\frac{1}{2}} \approx 4 \text{ d} \) on the soil surface (Herbicide Handbook 1989);  
\hspace{1cm} decomposed by sunlight, \( t_{\frac{1}{2}} = 25.7 \text{ min.} \) (Tomlin 1994).  
Oxidation:  
Hydrolysis: stable to hydrolysis between pH 4 and 10 at 40°C (Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).  
Biodegradation: slowly broken down by microorganisms in soil, in pure culture, a soil fungus metabolizes rapidly with \( t_{\frac{1}{2}} = 2 \text{ wk} \) (Herbicide Handbook 1989).  
Biotransformation: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).  
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:  
Half-Lives in the Environment:  
Air:  
Surface water:  
Ground water: decomposed by sunlight, \( t_{\frac{1}{2}} = 25.7 \text{ min.} \) (Montgomery 1993; Tomlin 1994).  
Sediment:  
Soil: \( t_{\frac{1}{2}} \approx 55 \text{ d} \) in the plots treated for the first time whereas \( t_{\frac{1}{2}} = 6–12 \text{ d} \) in pre-treated plots that had previously been sprayed with napropamide in the field; \( t_{\frac{1}{2}} = 25–40 \text{ d} \) irrespective of the pre-treatment history of the soil in the laboratory at 20°C (Walker & Welch 1992)  
\hspace{1cm} \( t_{\frac{1}{2}} \approx 8–12 \text{ wk} \) (Hartley & Kidd 1987; Tomlin 1994);  
\hspace{1cm} field \( t_{\frac{1}{2}} = 70 \text{ d} \) (Wauchope et al. 1992; Hornsby et al. 1996);  
\hspace{1cm} moist loam or sandy-loam soils at 79–90°C, \( t_{\frac{1}{2}} = 8–12 \text{ wk} \) (Montgomery 1993).  
Biota: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).
17.1.1.55 Neburon

Common Name: Neburon
Synonym: Kloben, Neburea, Neburex
Chemical Name: 1-butyl-3-(3,4-dichlorophenyl)-1-methylurea; N-butyl-N′(3,4-dichloro-phenyl)-N-methylurea

Uses: pre-emergence herbicide to control grasses and broadleaf weeds in peas, beans, lucerne, garlic, beets, cereals, strawberries, ornamentals and forestry.

CAS Registry No: 555-37-3
Molecular Formula: C_{12}H_{16}Cl_{2}N_{2}O
Molecular Weight: 275.174

Melting Point (°C):
- 102–103 (Khan 1980; Spencer 1982; Worthing & Hance 1991; Tomlin 1994)
- 101.5–103 (Montgomery 1993)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):
- 236.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
- 96.91 (Rordorf 1989)

Enthalpy of Fusion, ΔHₕₚ (kJ/mol):
- 29.71 (DSC method, Plato & Glasgow 1969)
- 26.9 (Rordorf 1989)

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 or as indicated):
- 4.8 (24°C, Bailey & White 1965; Melnikov 1971)
- 4.8 (Martin & Worthing 1977)
- 4.8 (28°C, Khan 1980)
- 5.0 (Hartley & Kidd 1987; Tomlin 1994)
- 5.2 (Spurlock 1992; Spurlock & Biggar 1994b)
- 5.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; selected, Hornsby et al. 1996)
- 4.67, 9.99 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 6.30 × 10⁻⁶, 4.10 × 10⁻⁴, 0.015, 0.33, 4.90 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (Pᵥ/Pₐ) = 18.272 – 6999.1/(T/K); measured range 50–103°C (solid, gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pₐ) = 13.285 – 5062.2/(T/K); measured range 105–140°C (liquid, gas saturation-GC, Rordorf 1989)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log Kᵥₚₒ:
- 4.59 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 4.31 (RP-HPLC-k’ correlation, Braumann et al. 1983)
- 4.22 (Spurlock 1992; Spurlock & Biggar 1994b)
- 3.80 (selected, Sangster 1993)
- 3.80 (calculated, Montgomery 1993)
Herbicides

4.10 (shake flask-UV, Liu & Qian 1995)
3.99 (RP-HPLC-k’ correlation, Liu & Qian 1995)
3.80 (recommended, Hansch et al. 1995)
3.40, 4.02, 4.13 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
2.41 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.85, 2.18 (calculated-S, K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
3.36 (soil, Hamaker & Thompson 1972)
3.26, 2.72 (soil, calculated-S, Kenaga 1980)
3.49 (average of soils/sediments, Rao & Davidson 1980)
3.36, 3.23 (quoted, calculated-MCI \chi, Gerstl & Helling 1987)
2.95 (soil, calculated-\chi and fragment contribution, Meylan et al. 1992)
3.49 (Montgomery 1993)
3.40 (selected, Lohninger 1994)
3.60 (calculated-K_{OC}, Liu & Qian 1995)
3.140 (soil, calculated-MCI 1\chi, Sabljic et al. 1995)
3.40; 2.86, 2.69 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Hydrolysis: t_{1/2} > 4 months for 5500 \mu g/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Half-Lives in the Environment:
Soil: residual activity in soil is limited to approximately 3–4 months (Hartley & Kidd 1987; quoted, Montgomery 1993); selected field t_{1/2} = 120 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
17.1.1.56 Nitralin

Common Name: Nitralin
Synonym: Planavin
Chemical Name: 4-(methylsulfonyl)-2,6-dinitro-N,N-dipropylbenzamine
CAS Registry No: 4726-14-1
Uses: herbicide
Molecular Formula: C_{13}H_{19}N_{3}O_{6}S
Molecular Weight: 345.371
Melting Point (°C): 150 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.39 (Hartley & Kidd 1987)
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
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: 0.0594 (mp at 150°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.60 (Melnikov 1971; Kenaga & Goring 1980; Kenaga 1980b; Isensee 1991)
0.60 (Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C):
0.240 (Ashton & Crafts 1981)
2.0 × 10⁻⁵ (Hartley & Kidd 1987)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:
6.73 (calculated-MCI χ, Patil 1994)
2.81 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF or log K_{b}:
2.90, 1.76 (calculated-solubility, K_{ow}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
2.98 (Kenaga & Goring 1980)
3.76 (calculated, Kenaga 1980a)
2.92 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.92; 3.28 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:
Biotransformation: Degradation by abiotic reductive transformations:
k = 3.44 M⁻¹ s⁻¹ in H₂S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:
k = 0.44 \times 10^{-3} \text{ h}^{-1} \text{ at pH 6.5, } k = 0.68 \times 10^{-2} \text{ h}^{-1} \text{ at pH 7.0, } k = 0.133 \text{ h}^{-1} \text{ at pH 7.4, and } k = 1.96 \text{ h}^{-1} \text{ at pH 7.8 for aqueous ferrous ion system;}

k = 0.580 \text{ h}^{-1} \text{ at pH 6.5, } k = 1.15 \text{ h}^{-1} \text{ at pH 6.7, } k = 6.06 \text{ h}^{-1} \text{ at pH 7.0, and } k = 20.9 \text{ h}^{-1} \text{ at pH 7.3 for Fe(II)/goethite system;}

k = 2.54 \times 10^{-3} \text{ h}^{-1} \text{ at pH 6.5, } k = 1.83 \times 10^{-3} \text{ h}^{-1} \text{ at pH 7.0, } k = 4.13 \times 10^{-3} \text{ h}^{-1} \text{ at pH 7.4 and } k = 7.70 \times 10^{-3} \text{ h}^{-1}

at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 \text{ mM(Wang & Arnold 2003)}

Half-Lives in the Environment:

- **Air:**
- **Surface water:**
- **Ground water:**
- **Sediment:**
- **Soil:** $t_{1/2} \approx 30$–$54$ d in dry soil (Hartley & Kidd 1987)
- **Biota:** in mammals, following oral administration, degradation and elimination occur within a few days (Hartley & Kidd 1987).
17.1.1.57 Nitrofen

Common Name: Nitrofen
Synonym: nitrophen Tok, Tokkron
Chemical Name: 2,4-dichloro-1-(4-nitrophenoxy)benzene
CAS Registry No: 1836-75-5
Uses: herbicide
Molecular Formula: C₁₂H₇Cl₂NO₃
Molecular Weight: 284.095
Melting Point (°C):
70 (Lide 2003)
Boiling Point (°C):
180–190/0.25 mmHg (Hartley & Kidd 1987)
Density (g/cm³ at 20°C):
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
93.66 (Rordorf 1989)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
22.7 (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: 0.362 (mp at 70°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):

1.0 (Kenaga 1980b)
~1.0 (Spencer 1982)
0.7–1.2 (22°C, Worthing 1987)
~1 (room temp., Hartley & Kidd 1987)
1.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

1.07 × 10⁻³ (40°C, Spencer 1982)
1.06 × 10⁻³ (40°C, Worthing 1987; Hartley & Kidd 1987)
1.30 × 10⁻¹, 4.50 × 10⁻³, 0.091, 1.20, 12.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 15.867 – 5886.5/(T/K); measured range 50–70.2°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 13.022 – 4892.8/(T/K); measured range 72.7–140°C (liquid, gas saturation-GC, Rordorf 1989)
1.33 × 10⁻⁵ (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m⁳/mol):
Octanol/Water Partition Coefficient, log \( K_{ow} \):
3.09 (Rao & Davidson 1980)
Octanol/Air Partition Coefficient, log \( K_{oa} \):
Bioconcentration Factor, log BCF or log \( K_{b} \):
2.79 (fish, Kenaga 1980b)
Sorption Partition Coefficient, log \( K_{oc} \):
3.64 (soil, calculated, Kenaga 1980b)
3.01, 3.64, 4.18, 4.05 (quoted literature values, Augustijn-Beckers et al. 1994)
4.0 (soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Herbicides

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

Half-Lives in the Environment:

Soil: reported field $t_{1/2} = 3$ to $25$ d and the recommended field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
17.1.1.58 Norflurazon

Common Name: Norflurazon
Synonym: Zorial, Solicam, Evital, Telok
Chemical Name: 4-chloro-5-(methylamino)-2[3-(trifluoromethyl)phenyl]-3-(2H)-pyridazinone
CAS Registry No: 27314-13-2
Uses: herbicide
Molecular Formula: C_{12}H_{9}ClF_{3}N_{3}O
Molecular Weight: 303.666
Melting Point (°C): 184 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pK_a:
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: 0.0275 (mp at 184°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 28 (Kenaga & Goring 1980; Kenaga 1980b; Gerstl & Helling 1987; Isensee 1991)
- 40 (Spencer 1982)
- 28 (23°C, Hartley & Kidd 1987)

Vapor Pressure (Pa at 25°C or as indicated):
- 2.7 × 10⁻⁶ (20°C, Ashton & Crafts 1981; Spencer 1982)
- 2.8 × 10⁻⁶ (20°C, Worthing & Walker 1987; Tomlin 1994)
- 2.7 × 10⁻⁶, 3.3 × 10⁻⁴, 3.3 × 10⁻³, 1.6 × 10⁻³, 1.3 × 10⁻² (20, 40, 60, 80, 100°C, Herbicide Handbook 1989)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

Octanol/Water Partition Coefficient, log K_{ow}:
- 2.30 (22°C, shake flask-UV, Braumann & Grimme 1981)
- 2.52 (shake flask, Takahashi et al. 1993)
- 2.45 (pH 6.5, Tomlin 1994)
- 2.30 (recommended, Hansch et al. 1995)
- 2.30 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
- 2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF or log K_{bi}:
- 1.97 (fish, calculated-solubility, Kenaga 1980b; Isensee 1991)
Sorption Partition Coefficient, log $K_{OC}$:

- 3.28 (soil, Kenaga & Goring 1980)
- 2.85 (calculated-solubility, Kenaga 1980b)
- 3.28, 3.07 (soil: quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
- 3.02, 2.64, 3.02, 2.46, 2.59 (sandy loam, Mississippi loam, Mississippi sediment, Keaton sandy loam, Biggs clay, Tomlin 1994)
- 3.75 (calculated-MCI $\chi$, Meylan et al. 1992)
- 3.28 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.78 (soil, Senseman et al. 1997)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization: dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45–180$ d (Tomlin 1994)

Photolysis: rapidly degraded by sunlight (Worthing 1987; Tomlin 1994)

dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45–180$ d (Tomlin 1994)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 3.4$ and $1.9$ d reported in the absence and presence of $20$ ppm $\text{H}_2\text{O}_2$ (quoted, Massad et al. 2004)

Ground water:

Sediment:

Soil: the average $t_{1/2} = 45–130$ d residues in soil from the Delta and Southeast depending on clay and organic content (Herbicide Handbook 1989)

field $t_{1/2} \sim 30$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996)

dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45–180$ d (Tomlin 1994)

soil $t_{1/2} = 90$ d (Senseman et al. 1997)

Biota:
17.1.1.59 Oryzalin

Common Name: Oryzalin
Synonym: Dirimal, EL 119, Rycel an, Ryzelan, Surflan
Chemical Name: 4-(dipropylamino)-3,5-dinitrobenzene-sulfonamide; 3,5-dinitro-\(N^4\), \(N^4\)-dipropylsulfanilamide
Uses: herbicide for pre-emergence control of many annual grasses and broadleaf weeds in cotton, fruit trees, vines, nut trees, soybeans, groundnuts, oilseed rape, sunflowers, lucerne, peas, sweet potatoes, mint, ornamentals and also used in noncrop areas.
CAS Registry No: 19044-88-3
Molecular Formula: \(C_{12}H_{18}N_4O_6S\)
Molecular Weight: 346.359
Melting Point (°C):
141 (Lide 2003)
Boiling Point (°C): 265 (dec. Tomlin 1994)
Density (g/cm\(^3\) at 20°C):
Molar Volume (cm\(^3\)/mol):
351.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant \(pK_a\):
8.60 (Wauchope et al. 1992; Hornsby et al. 1996)
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: 0.0728 (mp at 141°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
2.4 (Martin & Worthing 1977; Spencer 1982; Ashton & Crafts 1981)
2.6 (Weber et al. 1980)
2.5 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)
2.4 (Worthing & Walker 1987, Worthing & Hance 1991)
2.6 (Herbicide Handbook 1989; Tomlin 1994)
3.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)
Vapor Pressure (Pa at 25°C or as indicated):
< 1.33 \times 10^{-5} (30°C, Ashton & Crafts 1981)
< 1.30 \times 10^{-5} (30°C, Hartley & Kidd 1987)
< 1.33 \times 10^{-6} (Herbicide Handbook 1989; Tomlin 1994)
< 1.33 \times 10^{-5} (30°C, Budavari 1989)
< 1.30 \times 10^{-6} (Worthing & Hance 1991)
Henry’s Law Constant (Pa⋅m\(^3\)/mol at 25°C):
0.000188 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):
4.13 (selected, Dao et al. 1983)
3.73 (Worthing & Hance 1991)
Herbicides

3.72 (pH 7, Tomlin 1994)
3.73 (Milne 1995)
3.73 (selected, Hansch et al. 1995)
2.79 (MedChem master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
2.58 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log KOC:
3.43 (soil, calculated-S, Kenaga 1980)
2.78 (estimated-chemical structure, Lohninger 1994)
2.85–3.04 (Tomlin 1994)
3.40 (quoted or calculated-QSAR MCI \( \chi \), Sabljic et al. 1995)
3.40; 3.18 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Biodegradation: in soil, microbial degradation occurs rapidly, \( t_{1/2} = 2.1 \) months for aerobic and \( t_{1/2} = 10 \) d for anaerobic metabolism (Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field \( t_{1/2} = 20 \) d (Wauchope et al. 1992; Hornsby et al. 1996);
\[ t_{1/2} = 2.1 \text{ months for aerobic degradation and } t_{1/2} = 10 \text{ d for anaerobic degradation (Tomlin 1994).} \]
17.1.1.60 Pebulate

Common Name: Pebulate
Synonym: PEBC, R-2061, Stauffer 2061, Timmam-6-E
Chemical Name: S-propyl butylethyl(thiocarbamate); S-propyl butylethylcarbamothioate

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in tomatoes, sugar beet, and tobacco.

CAS Registry No: 1114-71-2
Molecular Formula: C_{10}H_{21}NOS
Molecular Weight: 203.345
Melting Point (°C): liquid
Boiling Point (°C):
142 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)
142 (at 21 mmHg, Herbicide Handbook 1989)
Density (g/cm³ at 20°C):
0.956 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
0.9555 (Herbicide Handbook 1989; Montgomery 1993)
Molar Volume (cm³/mol):
258.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

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):
92 (21°C, Woodford & Evans 1963)
92 (21°C, Spencer 1973, 1982)

Vapor Pressure (Pa at 25°C or as indicated):
3.60 (20°C, Hartley & Graham-Bryce 1980)
9.06 (30°C, Khan 1980)
0.216 (20°C, GC-RT correlation, Kim 1985)
9.00 (30°C, Hartley & Kidd 1987; Tomlin 1994)
3.50 (20°C, selected, Suntio et al. 1988)
4.70 (Worthing & Hance 1991; Tomlin 1994)
9.064 (20°C, Montgomery 1993)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
11.67 (20°C, calculated-P/C, Suntio et al. 1988)
11.65 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{ow}:
3.78 (selected, Magee 1991)
3.84 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Herbicides

3.83 (Tomlin 1994)
3.84 (selected, Hansch et al. 1995)
4.19, 3.74, 3.27 (RP-HPLC, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.79 (calculated-S, Kenaga 1980)
1.54 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.80 (soil, Hamaker & Thompson 1972)
2.66 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.80 (reported as log K_{OM}, Magee 1991)
2.65 (estimated as log K_{OM}, Magee 1991)
2.80 (Montgomery 1993)
2.63 (selected, Lohninger 1994)
2.80 (quoted or calculated-QSAR MCI χ, Sabljic et al. 1995)
2.48, 2.10 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Biodegradation: in soil, microbial degradation t_{1/2} = 2–3 wk (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: t_{1/2} = 11 d, at pH 4 and pH 10, t_{1/2} = 12 d at pH 7 (40°C, Tomlin 1994).
Ground water:
Sediment:
Soil: t_{1/2} ~ 2 wk in moist loam soil at 21–27°C (Herbicide Handbook 1989; Montgomery 1993);
selected field t_{1/2} = 14 d (Wauchope et al. 1992; Hornsby et al. 1996);
\( t_{1/2} = 2–3 \) wk (Tomlin 1994).

Biota:
17.1.1.61 Pendimethalin

![Chemical Structure of Pendimethalin]

Common Name: Pendimethalin
Synonym: penoxalin
Chemical Name: \(N\)-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine
CAS Registry No: 40487-42-1
Uses: herbicide
Molecular Formula: \(C_{13}H_{19}N_{3}O_{4}\)
Molecular Weight: 281.308
Melting Point (°C):
56 (Lide 2003)
Boiling Point (°C):
decomposes on heating (Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm\(^3\) at 25°C):
1.19 (Ashton & Crafts 1981; Montgomery 19993; Tomlin 1994)
1.12 (Hartley & Kidd 1987)
1.17 (Herbicide Handbook 1989)
Molar Volume (cm\(^3\)/mol):
Dissociation Constant \(\text{pK}_a\):
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: 0.496 (mp at 56°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
0.50 (23°C, Ashton & Crafts 1981)
0.30 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
0.275 (Herbicide Handbook 1989)
0.275 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.61 (20–25°C, Majewski & Capel 1995)
Vapor Pressure (Pa at 25°C or as indicated):
0.004 (Ashton & Crafts 1981; Herbicide Handbook 1989)
0.004 (Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)
0.004 (Montgomery 1993)
8.16 \times 10^{-3} (20–25°C, Majewski & Capel 1995)
0.00123; 0.00776 (liquid \(P_L\), GC-RT correlation; quoted lit., Donovan 1996)
Henry’s Law Constant (Pa-m\(^3\)/mol at 25°C or as indicated):
0.0867 (Montgomery 1993)
3.75 (20–25, calculated-P/C, Majewski & Capel 1995)
Octanol/Water Partition Coefficient, log \(K_{\text{ ow}}\):
5.18 (Montgomery 1993)
5.18 (Tomlin 1994)
5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
Herbicides

Octanol/Air Partition Coefficient, log $K_O/A$:

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_O/C$:
2.95  (soil, Wauchope et al. 1992; Hornsby et al. 1996)
4.20  (soil, Bottoni & Funari 1992)
4.14, 4.47  (loam, pH 7, pH 6.5, quoted, Montgomery 1993)
3.81  (sand, pH 7.6, Montgomery 1993)
4.07, 4.14  (sandy loam pH 6.4, silty loam, pH 7.0, Montgomery 1993)
1.48–2.93  (soil, Montgomery 1993)
3.70  (soil, Senseman et al. 1997)
3.14  (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: slowly decomposed by light (Hartley & Kidd 1987; Tomlin 1994).
Oxidation:
Hydrolysis: $t_{1/2} < 21$ d (Montgomery 1993).
Biodegradation: observed $t_{1/2} = 33$ d, 45 d, 52 d and 67 d in flooded and nonflooded conditions in nonsterile and sterile soils, respectively, in the study of degradation of pendimethalin under the influence of soil moisture and microbial activity in a sandy loam soil, in both nonsterile nonflooded and flooded soil, degradation followed first-order kinetics. (Kulshrestha & Singh 1992; quoted, Montgomery 1993).
Biotransformation: Degradation by abiotic reductive transformations:
$k = 1.25$ M$^{-1}$ s$^{-1}$ in H$_2$S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:
$k = 0.50 \times 10^{-3}$ h$^{-1}$ at pH 6.5, $k = 0.27 \times 10^{-2}$ h$^{-1}$ at pH 7.0, $k = 0.093$ h$^{-1}$ at pH 7.4, and $k = 0.81$ h$^{-1}$ at pH 7.8 for aqueous ferrous ion system;
$k = 0.216$ h$^{-1}$ at pH 6.5, $k = 0.274$ h$^{-1}$ at pH 6.7, $k = 0.918$ h$^{-1}$ at pH 7.0, and $k = 2.10$ h$^{-1}$ at pH 7.3 for Fe(II)/goethite system;
$k = 3.81 \times 10^{-3}$ h$^{-1}$ at pH 6.5, $k = 2.66 \times 10^{-3}$ h$^{-1}$ at pH 7.0, $k = 1.13 \times 10^{-2}$ h$^{-1}$ at pH 7.4 and $k = 1.74 \times 10^{-2}$ h$^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} < 21$ d in water (Tomlin 1994).
Ground water: reported $t_{1/2} = 30–90$ d (Bottoni & Funari 1992)
Sediment:
Soil: $t_{1/2} = 98$ and 409 d at 30 and 10°C in a sandy loam soil with 75% moisture (Walker & Bond 1977)
$t_{1/2} = 4$ d on Bosket silt loam, $t_{1/2} = 6$ d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2} = 18$ d on Bosket silt loam, $t_{1/2} = 27$ d on Sharkey clay (Savage & Jordon 1980)
$t_{1/2} = 58–63$ d in IARI sandy loam soil under Indian tropical climate (Kulshrestha & Yaduraju 1987)
$t_{1/2} = 30–90$ d or persistence (Bottoni & Funari 1992)
$t_{1/2} = 66.9$ d in sterile, $t_{1/2} = 52.2$ d in nonsterile non-flooded sandy loam soil; $t_{1/2} = 44.9$ d in sterile and 33.4 d in nonsterile flooded sandy loam soil in the study of degradation under the influence of soil moisture and microbial activity (Kulshrestha & Singh 1992; quoted, Montgomery 1993)
reported field $t_{1/2} = 8–480$ d, recommended $t_{1/2} = 90$ d (Wauchope et al. 1992; Hornsby et al. 1996); soil $t_{1/2} = 90$ d (Senseman et al. 1997).
Biota: $t_{1/2} = 3–4$ months (quoted, Hartley & Kidd 1987; Tomlin 1994)

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17.1.1.62 Picloram

Common Name: Picloram
Synonym: Amdon, ATCP, Borolin, Grazon, K-Pin, Tordon
Chemical Name: 4-amino-3,5,6-trichloropicolinic acid; 4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid
Uses: systemic herbicide to control most broadleaf weeds on grassland and noncropland.
CAS Registry No: 1918-02-1
Molecular Formula: C₆H₃Cl₃N₂O₂
Molecular Weight: 241.459
Melting Point (°C): 218.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   204.2 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)
Dissociation Constant pKₐ:
   1.90 (Weber et al. 1980; Willis & McDowell 1982)
   2.3 (22°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
   1.94 (Hornsby et al. 1996)
Enthalpy of Fusion, ∆Hₚₚ (kJ/mol):
Entropy of Fusion, ∆Sₚₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₚₚ = 56 J/mol K), F: 0.0126 (mp at 218.5°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):
   430 (Bailey & White 1965; Freed 1966; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Spencer 1982)
   546* (20°C, shake flask-IR, measured range 10–40°C, pH 2.8, distilled water, Cheung & Biggar 1974)
   73.65* (20°C, shake flask-IR, measured range 10–40°C at pH 0.2, Cheung & Biggar 1974)
   62.7* (20°C, shake flask-IR, measured range 10–40°C at pH 1.1, Cheung & Biggar 1974)
   137* (20°C, shake flask-IR, measured range 10–40°C at pH 2.0, Cheung & Biggar 1974)
   19560* (20°C, shake flask-IR, measured range 10–40°C at pH 4.2, Cheung & Biggar 1974)
   74593* (20°C, shake flask-IR, measured range 10–40°C at pH 4.7, Cheung & Biggar 1974)
   430 (Hartley & Graham-Bryce 1980; Taylor & Glotfelty 1988)
   400–430 (Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
   7.30 × 10⁻² (20°C, Hartley & Graham-Bryce 1980)
   9.70 × 10⁻⁹ (Dobbs & Cull 1982; quoted, Howard 1991)
   7.30 × 10⁻⁶ (20°C, quoted from Hartlet & Graham-Bryce 1980, Dobbs et al. 1984)
   6.00 × 10⁻³ (20°C, selected, Suntio et al. 1988)
4.50 × 10^{-8} (quoted, Nash 1989)
7.40 × 10^{-7} (20°C, selected, Taylor & Spencer 1990)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated):
4.20 × 10^{-7} (calculated-P/C, Taylor & Glotfelty 1988)
2.50 × 10^{-5} (calculated-P/C, Nash 1989)
4.10 × 10^{-6} (calculated-P/C, Howard 1991)
3.40 × 10^{-5} (20–35°C, calculated-P/C, Montgomery 1993)
3.17 × 10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
0.30 (Kenaga 1975)
0.63 (selected, Dao et al. 1983)
0.30 (Hansch & Leo 1985; Hansch et al. 1995;)
–3.47 (selected, Gerstl & Helling 1987)
1.166 (calculated as per Broto et al. 1984, Karcher & Devillers 1990)
0.26, 0.30 (quoted, Sangster 1993)
1.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
–1.70 (fish in static water, quoted from Dow Chemical data, Kenaga & Goring 1980)
1.30 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
–0.222 (calculated-K_{OC}, Kenaga 1980)
0.0 (estimated-K_{OC}, Lyman et al. 1982; quoted, Howard 1991)
1.49 (fish in flowing water, Garten & Trabalka 1983; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
1.23 (soil, Hamaker & Thompson 1972)
1.10 (average in soil, Hamaker & Thompson 1972)
1.10 (average in soil, Reinhold et al. 1979)
1.23 (Kenaga & Goring 1980; quoted, Bahnick & Doucette 1988)
2.20 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.41 (av. of 26 soils, Rao & Davidson 1980)
1.40 (soil, Rao & Davidson 1982)
1.31, 1.05, 1.34, 1.0, 1.26, 1.10, 1.05 (Catlin soil, Commerce soil, Fargo soil, Holdredge soil, Norfolk soil, Kawkawlin soil, Walla-Walla soil, McCall & Agin 1985; quoted, Brusseau & Rao 1989)
2.11 (calculated-MCI χ, Gerstl & Helling 1987)
1.68 (screening model calculations, Jury et al. 1987b)
1.47 (calculated-MCI χ, Bahnick & Doucette 1988)
1.88 (Nash 1989)
1.23 (reported as log K_{OM}, Magee 1991)
1.20 (organic carbon, Wauchope et al. 1991)
1.11, 1.41, 1.68 (soil, quoted values, Bottoni & Funari 1992)
1.41 (Montgomery 1993)
1.30 (soil, calculated-QSAR MCI χ, Sabljic et al. 1995)
1.55, 1.39, 2.38 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 2.0–10.5, average, Delle Site 2001)
3.07, 2.96, 3.30 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH ≤ 2.0 undissociated, average, Delle Site 2001)
1.80, 1.76 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 4.2–5.9, average, Delle Site 2001)
1.12, 2.02, 1.93 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, pH ≥ 6.0, dissociated, average, Delle Site 2001)
Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):

**Volatilization:**
- Photolysis:
  - \( t_{1/2} = 200 \) h for 40% of 4,840 \( \mu g/mL \) to degrade in dilute NaOH solution under sunlight (Hall et al. 1968; quoted, Cessna & Muir 1991);
  - \( t_{1/2} = 2.3 \) d to 9.58 d direct photolysis by sunlight under various conditions, at depths of 2.54 cm-3.65 m at various times of the year; one result at 3.65 m during Sept.-Oct. gave \( t_{1/2} = 41.3 \) d; distilled water and canal water gave essentially the same results in one set of experiments (Hedlund & Youngson 1972; quoted, Cessna & Muir 1991; Howard 1991);
  - \( t_{1/2} = 72 \) h for 99% of 548 \( \mu g/mL \) to degrade in Na salt solution under 300–380 nm light (Mosier & Guenzi 1973; quoted, Cessna & Muir 1991);
  - \( t_{1/2} = 0.5 \) h for 38% of 265 \( \mu g/mL \) to degrade in distilled water under 254 nm light (Glass 1975; quoted, Cessna & Muir 1991);
  - \( t_{1/2} = 2.2 \) d for < 2.4 \( \mu g/mL \) to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);
  - \( t_{1/2} = 16 \) h in surface water estimated from direct midday sunlight photolysis in mid-summer at 40\(^\circ\)N (Zepp 1991).

**Oxidation:**
- Photooxidation:
  - \( t_{1/2} = 12.21 \) d in air, based on estimated rate constant for the reaction with photochemically produced hydroxyl radical in the atmosphere (GEMS 1986; quoted, Howard 1991)
  - \( k = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \) for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 2.1–3.7 and at 24 ± 1°C (Buxton et al. 1988; quoted, Haag & Yao 1992)
  - \( k(\text{aq.}) = (50-150) \text{ M}^{-1} \text{ s}^{-1} \) for direct reaction with ozone in water at pH 1.5–4.9 and 21 ± 1°C, with \( t_{1/2} = 4.0 \) min at pH 7 (Yao & Haag 1991).
  - \( k(\text{aq.}) = (3.4 ± 0.3) \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \) for the reaction (Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 2.1–3.7 and at 24 ± 1°C (Haag & Yao 1992)
  - \( k(\text{aq.}) = 1.3 \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \) for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

**Hydrolysis:**
- Biodegradation:
  - \( t_{1/2} = 128–144 \) h in mixture of 5 g soil and 1–4 mL water, \( t_{1/2} = 90–1000 \) h in mixture of 1 mL water with 0.25–10 g soil, (Hance 1969; quoted, Howard 1991);
  - \( t_{1/2} > 15 \) months for 0.07, 0.72 and 10 \( \mu g/mL \) to biodegrade in groundwater (Weidner 1974; quoted, Muir 1991);
  - \( k = 0.0073 \text{ d}^{-1} \) by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);
  - biochemical \( t_{1/2} = 100 \) d from screening model calculations (Jury et al. 1987b);
  - \( t_{1/2} = 30–300 \) d, degraded slowly by soil microorganisms (Tomlin 1994).

**Biotransformation:**
- Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

**Half-Lives in the Environment:**

**Air:** \( t_{1/2} = 12.21 \) d, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (GEMS 1986; quoted, Howard 1991).

**Surface water:** \( t_{1/2} = 2.6 \) d decomposed by UV irradiation (Tomlin 1994);
  - measured rate constant \( k = (50 - 150) \text{ M}^{-1} \text{ s}^{-1} \) for direct reaction with ozone in water at pH 1.5–4.9 and 21°C, with \( t_{1/2} = 4.0 \) min at pH 7 (Yao & Haag 1991).

**Ground water:** \( t_{1/2} > 15 \) months for 0.07, 0.72 and 10 \( \mu g/mL \) to biodegrade in groundwater (Weidner 1974; quoted, Muir 1991);
  - measured rate constant \( k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1} \) for direct reaction with ozone in water at pH 2 and 21°C, with \( t_{1/2} \leq 80 \) d at pH 7 (Yao & Haag 1991)
  - reported \( t_{1/2} = 30–330, 138, 180 \) and 206 d (Bottoni & Funari 1992).

**Sediment:**
- Soil: estimated persistence of 18 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987b);
  - persistent in soils with \( t_{1/2} > 5 \) yr (Alexander 1973; quoted, Howard 1991);
  - estimated first-order \( t_{1/2} = 95 \) d in soil from biodegradation rate constant \( k = 0.0073 \text{ d}^{-1} \) by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);
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persistent in soil with \( t_{1/2} > 100 \text{ d} \) (Willis & McDowell 1982);
\( t_{1/2} = 100 \text{ d} \) from screening model calculations (Jury et al. 1987b);
selected \( t_{1/2} = 90 \text{ d} \) (Wauchope et al. 1991; quoted, Dowd et al. 1993);
reported \( t_{1/2} = 30–330 \text{ d}, 18 \text{ d}, 180 \text{ d} \) and 206 d (Bottoni & Funari 1992);
\( t_{1/2} = 3–330 \text{ d} \) (Tomlin 1994).

Biota: biochemical \( t_{1/2} = 100 \text{ d} \) from screening model calculations (Jury et al. 1987b);
average \( t_{1/2} = 60 \text{ d} \) in the forest (USDA 1989; quoted, Neary et al. 1993).

### TABLE 17.1.1.62.1

Reported aqueous solubilities of picloram at various temperatures

Cheung & Biggar 1974

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \text{S/g·m}^-3 )</th>
<th>( \text{S/g·m}^-3 )</th>
<th>( \text{S/g·m}^-3 )</th>
<th>( \text{S/g·m}^-3 )</th>
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<td>pH 2.8</td>
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<td>pH 4.2</td>
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<td>pH 4.7</td>
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</table>

\( \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) \) 38.49 38.91 31.38 12.97 0 0
### 17.1.1.63 Profluralin

![Chemical Structure](image)

- **Common Name:** Profluralin  
- **Synonym:** CGA 10832, Pregard, Tolban  
- **Chemical Name:** $N$-(cyclopropylmethyl)-2,6-dinitro-$N$-propyl-4-trifluoromethylaniline; $N$-(cyclopropylmethyl)-2,6-dinitro-$N$-propyl-4-(trifluoromethyl) benzenamine  

**Uses:** herbicide for pre-planting by soil incorporation to control annual and perennial broadleaf and grass weeds in cotton, soybeans, brassicas, capsicums, tomatoes and other crops.

**CAS Registry No:** 26399-36-0  
**Molecular Formula:** $C_{14}H_{16}F_{3}N_{3}O_{4}$  
**Molecular Weight:** 347.290  
**Melting Point (°C):** 34 (Lide 2003)  
**Boiling Point (°C):**  
- 1.45 (25°C, Ashton & Crafts 1981)  
- 1.38 (Hartley & Kidd 1987; Worthing & Hance 1991)  
**Molar Volume (cm$^3$/mol):** 304.7 (calculated-Le Bas method at normal boiling point)  
**Dissociation Constant pK$_a$:**  
**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:** 0.816 (mp at 34°C)  
**Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):**  
- 0.10 (20°C, Weber 1972)  
- 0.10 (Spencer 1973, 1982; Wauchope 1978; Kenaga 1980)  
- 0.10 (27°C, Ashton & Crafts 1973, 1981)  
- 0.10 (shake flask-HPLC, Ellgehausen et al. 1981)  
- 0.10 (20°C, Hartley & Kidd 1987; Milne 1995)  
- 0.10 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)  
- 0.10 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
- 0.0092 (20°C, Weber 1972; Worthing & Walker 1987)  
- 0.0084 (20°C, Hartley & Kidd 1987)  
- 0.0084 (20°C, Worthing & Hance 1991)  
- 0.0084 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
**Henry’s Law Constant (Pa·m$^3$/mol at 25°C or as indicated):**  
- 31.91 (20°C, calculated-P/C, Muir 1991)  
**Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:**  
- 5.16 (selected, Dao et al. 1983)  
- 6.34 (shake flask-HPLC/UV, Ellgehausen et al. 1981)  
- 6.34 (recommended, Sangster 1993)
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Bioconcentration Factor, log BCF:
- 3.35 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 2.83 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
- 3.93 (soil, expl., Kenaga 1980)
- 4.19 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 3.83 (estimated as log K_{OM}, Magee 1991)
- 3.93 (soil, quoted expl., Meylan et al. 1992)
- 4.26 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 4.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 4.16 (selected, Lohninger 1994)
- 4.01 (soil, calculated-QSAR MCI 1χ and fragment contribution, Sabljic et al. 1995)
- 3.87 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
- Volatilization: estimated t_{1/2} ~ 1.2 d from 1 m depth of water at 20°C (Muir 1991).
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biodegradation: t_{1/2} = 12 d for 0.5 µg mL^{-1} to biodegrade in flooded soils at 20–42°C (Savage 1978; quoted, Muir 1991);
  - Degradation t_{1/2} < 1 month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm profluralin) for 4 month under aerobic conditions, no degradation in sterile controls.
  - (shake flask-TLC, Camper et al. 1980)
  - t_{1/2} < 1 month for 1 µg/mL to biodegrade in flooded soils at 25°C (derived from results of Camper et al. 1980, Muir 1991);
  - biodegradation t_{1/2} < 20 d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).
- Biotransformation:
  - Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:

Half-Lives in the Environment:
- Air:
  - Surface water: biodegradation t_{1/2} < 20 d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).
- Ground water:
  - Sediment: biodegradation t_{1/2} < 20 d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).
- Soil: t_{1/2} = 12 d for 0.5 µg mL^{-1} to biodegrade in flooded soils at 20–42°C (Savage 1978, Muir 1991)
  - persistence of 12 months in soil (Wauchope 1978);
  - aerobic and anaerobic degradation t_{1/2} < 1 month in 3 flooded soils at 25°C (Camper et al. 1980);
  - field studies, t_{1/2} = 10.9 wk - 1978 first study; t_{1/2} = 10.1 wk - 1978 second study; t_{1/2} = 11.5 wk - 1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)
  - laboratory studies: t_{1/2} = 19.9 wk at 4°C, t_{1/2} = 6.7 wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt loam), t_{1/2} = 20.4 wk at 4°C, t_{1/2} = 4.8 wk at 25°C for flooded soils, Crowley silt loam; and t_{1/2} = 25.8 wk at 4°C, t_{1/2} = 8.6 wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay), t_{1/2} = 21.3 wk at 4°C and t_{1/2} = 6.2 wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982);
  - selected field t_{1/2} = 110 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:
17.1.1.64 Prometon

Common Name: Prometon
Synonym: G 31435, Gesafram, Gesagram, Methoxypropazine, Ontracic 800, Ontrack, Pramitol, Prometone
Chemical Name: 6-methoxy-N,N′-bis(methylethyl)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-methoxy-1,3,5-triazine
Uses: nonselective pre-emergence and post-emergence herbicide to control most annual and broadleaf weeds, grasses, and brush weeds on noncropland.
CAS Registry No: 1610-18-0
Molecular Formula: \( \text{C}_{10}\text{H}_{19}\text{N}_{5}\text{O} \)
Molecular Weight: 225.291
Melting Point (°C): 91.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.088 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
Molar Volume (cm³/mol):
280.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
- 4.28 \( (pK_a, \text{Weber 1970; quoted, Bintein & Devillers 1994}) \)
- 4.30 \( (pK_a, 21^\circ\text{C}, \text{Worthing & Hance 1991; Montgomery 1993}) \)
- 9.73 \( (pK_a, \text{Wauchope et al. 1992; Hornsby et al. 1996}) \)
- 9.7 \( (21^\circ\text{C}, pK_a, \text{Tomlin 1994}) \)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
90.77 \( (\text{Rordorf 1989}) \)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
22.175 \( (\text{DSC method, Plato & Glasgow 1969}) \)
21.6 \( (\text{Rordorf 1989}) \)
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \text{ J/mol K} \)), F: 0.223 (mp at 91.5°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 750 \( (20^\circ\text{C}, \text{Bailey & White 1965; Ashton & Crafts 1981; Herbicide Handbook 1989}) \)
- 1000, 678, 669 \( (26^\circ\text{C}, \text{pH 3.0, 7.0, 10.0, shake flask-UV, Ward & Weber 1968}) \)
- 750 \( (\text{Martin & Worthing 1977; Herbicide Handbook 1978}) \)
- 677 \( (\text{Weber et al. 1980}) \)
- 620 \( (20^\circ\text{C}, \text{Spencer 1982}) \)
- 750 \( (20^\circ\text{C}, \text{Verschueren 1983}) \)
- 750 \( (20^\circ\text{C}, \text{Hartley & Kidd 1987; Montgomery 1993}) \)
- 620 \( (20^\circ\text{C}, \text{Worthing & Walker 1987, 1991; Tomlin 1994}) \)
- 720 \( (20–25^\circ\text{C}, \text{selected, Wauchope et al. 1992; Hornsby et al. 1996}) \)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
- \( 3.07 \times 10^{-4} \) \( (20^\circ\text{C}, \text{extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964}) \) (See figure at the end of this section.)
- \( \log (P/\text{mmHg}) = 11.911 – 4933/(T/\text{K}) \), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964)
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0.00030 (20°C, Khan 1980)
0.00031 (20°C, Ashton & Crafts 1981; Worthing & Hance 1991)
0.00083 (Jury et al. 1984; selected, Spencer et al. 1988; Spencer & Cliath 1990; Taylor & Spencer 1990)
0.00031 (20°C, Hartley & Kidd 1987)
0.00031, 0.00105 (20°C, 30°C, Herbicide Handbook 1989)
0.00031, 0.00105 (20°C, 30°C, Herbicide Handbook 1989)
1.0 × 10⁻⁵, 3.30 × 10⁻², 0.65, 8.60, 82 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 16.525 − 5817.4/(T/K); measured range 32.1–89.3°C (gas saturation-GC, Rordorf 1989)
log (P/Pa) = 13.617 − 4741.7/(T/K); measured range 92.3–140°C (gas saturation-GC, Rordorf 1989)
0.00031 (20°C, Montgomery 1993)
0.000306 (20°C, Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
2.50 × 10⁻⁴ (calculated-P/C, Jury et al. 1984; Spencer et al. 1988; Spencer & Cliath 1990)
9.02 × 10⁻³ (20°C, calculated-P/C, Montgomery 1993)
9.01 × 10⁻³ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.94 (selected, Dao et al. 1983)
1.94 (Gerstl & Helling 1987)
2.99 (RP-HPLC-RT correlation, Finizio et al. 1991; quoted, Sangster 1993)
2.85 (selected, Magee 1991)
2.55 (shake flask-UV, Liu & Qian 1995)
2.69, 2.99 (Montgomery 1993)
2.99 (recommended, Hansch et al. 1995)
2.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.28 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.54 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.04 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.61 (Jury et al. 1984; quoted, Spencer & Cliath 1990)
2.40 (calculated-MCI χ, Gerstl & Helling)
2.48 (Spencer et al. 1988)
2.35 (estimated as log K_{OM}, Magee 1991)
2.20 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.92–2.24 (Montgomery 1993)
2.77 (selected, Lohninger 1994)
2.39 (calculated-K_{OM}, Liu & Qian 1995)
2.50 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.60; 2.70, 2.68 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.47, 2.50 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 4.3–7.1, average, Delle Site 2001)
2.81, 2.65, 2.53 (soils with organic carbon OC ≥ 0.5% at: pH 4.3–4.9, pH 5.0–5.9, pH- 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, or Half-Lives, t_{1/2}:
Volatile: estimated t_{1/2} ~ 100 d (Spencer & Cliath 1990).
Photolysis: t_{1/2} = 2.25 h for 1% of 100 µg mL⁻¹ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).
Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \( k_1 \) and Elimination \( k_2 \) Rate Constants:

Half-Lives in the Environment:

Soil: selected field \( t_{1/2} = 500 \) d (Wauchope et al. 1992; Hornsby et al. 1996).

**FIGURE 17.1.1.64.1** Logarithm of vapor pressure versus reciprocal temperature for prometon.
17.1.1.65 Prometryn

Common Name: Prometryn

Synonym: Caparol, Cotton-Pro, Gesagard, G-34161, Mercasin, Mercazin, Polisin, Primatol, Prometrex, Prometrin, Selectin, Sesagard, Uvon

Chemical Name: $\text{N,N}^\prime$-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-(methylthio)-1,3,5-triazine

Uses: selective herbicide to control many annual grass and broadleaf weeds in celery, cotton and peas.

CAS Registry No: 7287-19-6

Molecular Formula: $\text{C}_{10}\text{H}_{19}\text{N}_{5}\text{S}$

Molecular Weight: 241.357

Melting Point (°C): 119 (Lide 2003)


Density (g/cm³ at 20°C): 299.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.05 (pKₐ, Weber 1970; Pacakova et al. 1988; Somasundaram et al. 1991; Bintein & Devillers 1994)


4.05 (pKₐ, 21°C, Montgomery 1993)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):

96.43 (Rordorf 1989)

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):

26.36 (DSC method, Plato & Glasgow 1969)

25.4 (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: 0.120 (mp at 119°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

48 (20°C, Woodford & Evans 1963)


206, 40.3, 41.8 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

48 (Martin & Worthing 1977; Herbicide Handbook 1978)

40 (Weber et al. 1980)


33 (Tomlin 1994; selected, Lohninger 1994)

241 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

$1.33 \times 10^{-4}$ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964)
0.00028 (from Friedrich & Stammbach 1964; Jury et al. 1983; 1984; Spencer & Cliath 1990)
0.00013 (20°C, Ashton & Crafts 1973, 1981)
0.00013 (20–25°C, Weber et al. 1980)
0.00028 (quoted, Jury et al. 1984; Spencer & Cliath 1990)
0.00013 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
0.00010 (20°C, selected, Suntio et al. 1988)
0.00013, 0.00053 (20, 30°C, Herbicide Handbook 1989)
1.60 × 10⁻⁴, 6.70 × 10⁻³, 0.16, 2.50, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
\[ \log \left( \frac{P}{Pa} \right) = 17.063 - 6215.6/(T/K); \text{measured range 32.4–117°C (gas saturation-GC, Rordorf 1989)} \]
\[ \log \left( \frac{P}{Pa} \right) = 14.013 - 5037.2/(T/K); \text{measured range 129–140°C (gas saturation-GC, Rordorf 1989)} \]
0.00017 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.000169 (Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.00139 (calculated-P/C, Jury et al. 1984; quoted, Spencer & Cliath 1990)
0.00139 (calculated-P/C, Jury et al. 1987a,b; Jury & Ghodrati 1989)
0.00050 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
0.00050 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
2.99 (selected, Dao et al. 1983)
1.91 (RP-HPLC-k’ correlation, Braumann et al. 1983)
3.46 (selected, Yoshioka et al. 1986)
3.51 (shake flask, Mitsutake et al. 1986)
2.99 (Gerstl & Helling 1987)
3.34 (RP-HPLC-RT correlation, Finizio et al. 1991)
3.43 (selected, Magee 1991)
3.34 (Worthing & Hance 1991; Milne 1995)
3.34, 3.46 (Montgomery 1993)
3.51 (recommended, Sangster 1993)
2.93 (RP-HPLC-k’ correlation, Liu & Qian 1995)
3.51 (recommended, Hansch et al. 1995)
3.35 (Pomona-database, Müller & Kördel 1996)
3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)
2.99 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.85, 1.67 (calculated-S, \( K_{\text{OC}} \), Kenaga 1980)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):
2.91 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.72 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.79 (Rao & Davidson 1980)
3.17 (calculated-MCI \( \chi \), Gerstl & Helling)
2.78 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
2.75 (estimated as log \( K_{\text{OM}} \), Magee 1991)
2.72–2.91, 2.79, 2.83 (soil, quoted values, Bottoni & Funari 1992)
2.38 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.28–2.79 (Montgomery 1993)
3.15 (estimated-chemical structure, Lohninger 1994)
2.60 (soil, Tomlin 1994)
2.63 (calculated-\( K_{\text{OW}} \), Liu & Qian 1995)
2.85 (soil, calculated-QSAR MCI \( \chi \), Sabljic et al. 1995)
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2.38; 2.84 (HPLC-screening method; calculated-PECOC fragment method, Müller & Kördel 1996)
3.54, 1.595, 1.968, 1.77, 2.67 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibration-HPLC/UV, Gawlik et al. 1998)
3.24, 2.16, 2.86, 2.59, 2.53 (calculated-Kow; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.544, 2.635, 2.484, 1.816, 2.933 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibration-HPLC/UV and HPLC-k correlation, Gawlik et al. 2000)
2.85, 2.89 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t1/2:

Volatilization: t1/2 = 60 d (Jury et al. 1984).
Photolysis:
Oxidation:
Hydrolysis: t1/2 = 22 d in 0.1 N hydrochloric acid solution, t1/2 = 500 yr at pH 7 in distilled water and t1/2 = 30 yr in 0.01 sodium hydroxide solution all at 25°C (Montgomery 1993).
Biodegradation: t1/2 = 60 d (Wauchope 1978);
t1/2 = 60 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1987a,b; Jury & Ghodrati 1989);
soil microbial degradation t1/2 = 70 d (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: completely decomposed when exposed to UV light for 3 h (Montgomery 1993).
Ground water: reported half-lives or persistence, t1/2 = 40–70, 60 and 94 d (Bottoni & Funari 1992)
Sediment:
Soil: estimated persistence of 3 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a,b; Jury & Ghodrati 1989);
t1/2 ~ 6 months to biodegrade in flooded soils (Plimmer et al. 1970; quoted, Muir 1991);
persistence of 2 months in soil (Wauchope 1978);
reported t1/2 = 40–70 d, 60 d and 94 d (Bottoni & Funari 1992);
selected field t1/2 = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);
t1/2 = 70 d for microbial degradation in soil (Tomlin 1994).
Biota: biochemical t1/2 = 60 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

FIGURE 17.1.165.1 Logarithm of vapor pressure versus reciprocal temperature for prometryn.
17.1.1.66 Pronamide

Common Name: Pronamide
Synonym: Kerb, Promamide, Propyzamide, RH-315
Chemical Name: 3,5-dichloro-N-(1,1-dimethylpropynyl)benzamide
Uses: herbicide.
CAS Registry No: 23950-58-5
Molecular Formula: C₁₂H₁₁Cl₂NO
Molecular Weight: 256.127
Melting Point (°C): 155 (Lide 2003)
Boiling Point (°C): 321
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
270.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 0.0530 (mp at 155°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
15 (15°C, Khan 1980)
15 (Ashton & Crafts 1981)
15 (Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
0.0113 (Khan 1980)
0.0536 (Dixon & Rissman 1985; quoted, Howard 1991)
0.227 (Worthing & Walker 1987)
0.0113 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.000058 (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.912 (Dixon & Rissman 1985)
0.193 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
0.188 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log KₐW:
3.26 (estimated, Lyman et al. 1982; quoted, Howard 1991)
3.36 (selected, Magee 1991)
3.26 (selected, Dao et al. 1983)
2.95 (estimated-QSAR and SPARC, Kollig et al. 1993)
3.09–3.28 (Tomlin 1994; Milne 1995)
3.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Bioconcentration Factor, log BCF:

- 2.13 (calculated-S, Kenaga 1980)
- 1.00 (calculated-$K_{OC}$, Kenaga 1980)
- 2.25 (estimated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1991)
- 2.13 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)

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

- 2.30 (soil, Leistra et al. 1974; Carlson et al.)
- 2.30 (measured for single soil, Kenaga 1980)
- 3.00 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.99 (soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
- 2.30; 2.42 (reported as log $K_{OM}$, estimated as log $K_{OM}$, Magee 1991)
- 2.30; 3.20 (soil, quoted; calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 2.63 (estimated-QSAR and SPARC, Kollig 1993)
- 2.54 (selected, Lohninger 1994)
- 2.31 (soil, calculated-QSAR MCI $\chi$, Sabljic et al. 1995)

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

- Volatilization: based on a Henry's law constant of 0.9118 Pa·m$^3$/mol, $t_{1/2} \sim 6.6$ d from a river 1-m deep flowing 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991).
- Photolysis: degraded photolytically on soil thin films, $t_{1/2} = 13–57$ d in artificial sunlight (Tomlin 1994).
- Oxidation: photooxidation $t_{1/2} = 4.2$ h in air, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).
- Hydrolysis: neutral hydrolysis rate constant $k < 1.5 \times 10^{-5}$ h$^{-1}$ with a calculated $t_{1/2} > 700$ d in neutral solution and with faster hydrolysis rates in acidic and basic solutions to be expected (Ellington et al. 1987, 1988; quoted, Howard 1991).
- Biodegradation: depending on soil and climatic conditions, the degradation $t_{1/2} = 10$ to 112 d, but a $t_{1/2} = 40$ d may be more common under field conditions (Walker 1976, 78; Zandvoort et al. 1979; quoted, Howard 1991).
- Biotransformation: second-order rate constant $k = 5 \times 10^{-14}$ L/organisms·h with an estimated $t_{1/2} \sim 580$ d for microbial degradation in natural water (Steen & Collette 1989; quoted, Howard 1991).

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

Half-Lives in the Environment:

- Air: $t_{1/2} = 4.2$ h, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).
- Surface water:
- Ground water:
- Sediment:
- Soil: depending on soil and climatic conditions, the degradation $t_{1/2} = 10$ to 112 d, but a $t_{1/2} = 40$ d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991);
- selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);
- degraded photolytically on soil thin films, $t_{1/2} = 13–57$ d in artificial sunlight (Tomlin 1994).

Biota:
17.1.1.67 Propachlor

![Propachlor molecule](image)

Common Name: Propachlor
Synonym: Albrass, Bexton, CIPA, CP 31393, Niticid, Propachlore, Prolex, Ramrod, Satecid
Chemical Name: 2-chloro-N-(1-methylethyl)-N-phenylacetamide; 2-chloro-N-isopropyl acetanilide
Uses: selective pre-emergence herbicide to control most annual grasses and some broadleaf weeds in brassicas, corn, cotton, flax, leeks, maize, milo, onions, peas, roses, ornamental trees and shrubs, soybeans, and sugar cane.
CAS Registry No: 1918-16-7
Molecular Formula: C_{11}H_{14}ClNO
Molecular Weight: 211.688
Melting Point (°C):
Boiling Point (°C):
110 (at 0.03 mmHg, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
231.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ∆H_{ fus} (kJ/mol):
27.614 (DSC method, Plato 1972)
Entropy of Fusion, ∆S_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{ fus} = 56 J/mol K), F: 0.309 (mp at 77°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
700 (Melnikov 1971; Khan 1980)
614 (20°C, Weber 1972)
693 (Spencer 1973, 1982)
580 (20°C, Ashton & Crafts 1973)
580 (Martin & Worthing 1977; Herbicide Handbook 1978)
839 (generator column-HPLC-RI, Swann et al. 1983)
2300 (HPLC-RT correlation, Swann et al. 1983)
613–700 (Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
0.032 (20–25°C, Weber et al. 1980)
0.0307 (24°C, Beestman & Demming 1974)
0.03 (Hartley & Kidd 1987)
0.03 (20°C, selected, Suntio et al. 1988)
0.0306 (Worthing & Hance 1991; Tomlin 1994)
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0.0307 \( (20–25^\circ C, \) selected, Wauchope et al. 1992; Hornsby et al. 1996) \\
0.03 \( (\) Montgomery 1993 \( ) \)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.011 \( (20^\circ C, \) calculated-P/C, Suntio et al. 1988) \\
0.011 \( (20^\circ C, \) calculated-P/C, Muir 1991) \\
0.011 \( (\) calculated-P/C, Montgomery 1993 \( ) \)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
2.75 \( (\) Leo et al. 1971 \( ) \)
1.61 \( (\) Rao & Davidson 1980 \( ) \)
2.80 \( (\) selected, Gerstl & Helling 1987 \( ) \)
2.18 \( (\) shake flask, Log P Database, Hansch & Leo 1987 \( ) \)
2.18 \( (\) selected, Magee 1991 \( ) \)
1.61 \( (\) Montgomery 1993 \( ) \)
2.18 \( (\) recommended, Sangster 1993 \( ) \)
1.62–2.30 \( (\) Tomlin 1994 \( ) \)
2.18 \( (\) recommended, Hansch et al. 1995 \( ) \)
2.36 \( (\) RP-HPLC-RT correlation, Finizio et al. 1997 \( ) \)
2.88 ± 0.17, 2.86 ± 0.12 \( (\) isocratic RP-HPLC-k’ correlation, gradient RP-HPLC-k’ correlation, Paschke et al. 2004 \( ) \)

Bioconcentration Factor, log BCF:
1.23 \( (\) calculated-S, Kenaga 1980 \( ) \)
1.15 \( (\) calculated-K_{\text{OC}}, Kenaga 1980 \( ) \)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):
2.42 \( (\) soil, Beestman & Demming 1976; Kenaga 1980; Kenaga & Goring 1980 \( ) \)
2.11 \( (\) soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980 \( ) \)
2.43 \( (\) calculated-MCI \( \chi \), Gerstl & Helling 1987 \( ) \)
2.62 \( (\) screening model calculations, Jury et al. 1987b \( ) \)
2.31 \( (\) estimated as log \( K_{\text{OM}} \), Magee 1991 \( ) \)
2.45 \( (\) soil, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992 \( ) \)
1.90 \( (\) soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996 \( ) \)
2.07–2.11 \( (\) Montgomery 1993 \( ) \)
2.62 \( (\) estimated-chemical structure, Lohninger 1994 \( ) \)
2.42 \( (\) quoted or calculated-QSAR MCI \( \chi \), Sabljic et al. 1995 \( ) \)
2.18 \( (\) soil, estimated-general model using molecular descriptors, Gramatica et al. 2000 \( ) \)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{\text{1/2}} \):
Volatilization: estimated \( t_{\text{1/2}} = 671 \) d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: \( t_{\text{1/2}} = 2.25 \) h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
1 ppb contaminated water in the presence of TiO₂ and H₂O₂ completely photodegraded after 3 h by solar irradiation (Muszkat et al. 1992).
Oxidation:
Hydrolysis:
Biodegradation: \( t_{\text{1/2}} \mu 10–14 \) d for 0.001–1.0 \( \mu \)g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991);
biological \( t_{\text{1/2}} = 7 \) d from screening model calculations (Jury et al. 1987b).
Biotransformation: second-order microbial rate constant \( k = 1.1 \times 10^{-9} \) L·organisms⁻¹ h⁻¹ (Steen & Collette 1989).
Bioconcentration, Uptake (\( k_{\text{1}} \)) and Elimination (\( k_{\text{2}} \)) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: \( t_{\text{1/2}} \sim 10–14 \) d for 0.001–1.0 \( \mu \)g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991).
Ground water:

Sediment:

Soil: persistence of 2 months (Wauchope 1978);

\[ t_{1/2} = 7 \text{ d from screening model calculations} \text{ Jury et al. 1987b}; \]

persists in soil for 28–42 d (Worthing & Hance 1991);

selected field \( t_{1/2} = 6.3 \text{ d (Wauchope et al. 1992; Hornsby et al. 1996).} \)

Biota: biochemical \( t_{1/2} = 7 \text{ d from screening model calculations (Jury et al. 1987b).} \)
17.1.1.68 Propanil

Common Name: Propanils
Chemical Name: \( N-(3,4\text{-dichlorophenyl})\text{propionamide; } N-(3,4\text{-dichlorophenyl})\text{propanamide} \)
Uses: selective emergence and post-emergence herbicide to control many grasses and broadleaf weeds in potatoes, rice and wheat.
CAS Registry No: 709-98-8
Molecular Formula: \( C_9H_9Cl_2NO \)
Molecular Weight: 218.079
Melting Point (°C):
\[ 92 \text{ (Lide 2003)} \]
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
\[ 1.41 \text{ (22°C, Tomlin 1994)} \]
Molar Volume (cm\(^3\)/mol):
\[ 220.1 \text{ (calculated-Le Bas method at normal boiling point)} \]
Dissociation Constant \( pK_a \):
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
\[ 95.1 \text{ (Rordorf 1989)} \]
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
\[ 20.08 \text{ (DSC method, Plato & Glasgow 1969)} \]
\[ 15.3 \text{ (Rordorf 1989)} \]
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: 0.220 (mp at 92°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
\[ 225 \text{ (Woodford & Evans 1963; Khan 1980)} \]
\[ 500 \text{ (Bailey & White 1965; Ashton & Crafts 1973; Herbicide Handbook 1989)} \]
\[ 268 \text{ (Freed 1966)} \]
\[ 225 \text{ (Martin & Worthing 1977; Worthing & Walker 1987; Herbicide Handbook 1983)} \]
\[ 268-500 \text{ (Weber et al. 1980)} \]
\[ 130 \text{ (20°C, Spencer 1982)} \]
\[ 225 \text{ (Hartley & Kidd 1987; Milne 1995)} \]
\[ 130 \text{ (20°C, Worthing & Hance 1991)} \]
\[ 200 \text{ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)} \]
\[ 130, 225 \text{ (20°C, 25°C, Montgomery 1993)} \]
\[ 130 \text{ (Tomlin 1994)} \]
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
\[ 0.012 \text{ (60°C, Khan 1980)} \]
\[ 0.012 \text{ (60°C, Verschueren 1983)} \]
\[ 0.012 \text{ (60°C, Hartley & Kidd 1987)} \]
\[ 0.005 \text{ (20°C, selected, Suntio et al. 1988)} \]
\[ 2.50 \times 10^{-4}, 7.20 \times 10^{-3}, 0.130, 1.50, 13.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)} \]
\[
\log \left( \frac{P}{P_a} \right) = 15.201 - 5604.1/(T/K); \text{ measured range 36.4–92.6°C (gas saturation-GC, Rordorf 1989)}
\]
\[
\log \left( \frac{P}{P_a} \right) = 13.192 - 4863.1/(T/K); \text{ measured range 95.1–160°C (gas saturation-GC, Rordorf 1989)}
\]
\[
2.60 \times 10^{-5} \quad (20^\circ C, \text{ Worthing & Hance 1991})
\]
\[
0.00533 \quad (20–25^\circ C, \text{ selected, Wauchope et al. 1992; Hornsby et al. 1996})
\]
\[
2.67 \times 10^{-5} \quad (20^\circ C, \text{ Montgomery 1993})
\]

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

\[
0.0036 \quad (20^\circ C, \text{ calculated-P/C, Suntio et al. 1988})
\]
\[
0.0036 \quad (20^\circ C, \text{ calculated-P/C, Montgomery 1993})
\]
\[
0.00545 \quad (\text{calculated-P/C, this work})
\]

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

\[
2.02 \quad (\text{Rao & Davidson 1980})
\]
\[
2.80 \quad (20 \pm 2^\circ C, \text{ shake flask-UV, Briggs 1981})
\]
\[
3.12 \quad (\text{selected, Dao et al. 1983})
\]
\[
3.07 \quad (\text{shake flask, Log P Database, Hansch & Leo 1987})
\]
\[
2.99 \quad (\text{selected, Gerstl & Helling 1987})
\]
\[
2.29 \quad (\text{Worthing & Hance 1991; Milne 1995})
\]
\[
2.34 \quad (\text{quoted from Kenaga 1980, Bottoni & Funari 1992})
\]
\[
2.73 \quad (\text{RP-HPLC-RT correlation, Sicbaldi & Finizio 1993})
\]
\[
2.03, 2.29 \quad (\text{Montgomery 1993})
\]
\[
3.07 \quad (\text{recommended, Sangster 1993})
\]
\[
2.80 \quad (\text{RP-HPLC-RT correlation, Saito et al. 1993})
\]
\[
3.30 \quad (\text{Tomlin 199})
\]
\[
3.07 \quad (\text{selected, Hansch et al. 1995})
\]
\[
2.73 \quad (\text{RP-HPLC-RT correlation, Finizio et al. 1997})
\]
\[
3.21 \quad (\text{RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002})
\]

Bioconcentration Factor, log \( BCF \):

\[
1.46 \quad (\text{calculated-S, Kenaga 1980})
\]
\[
1.34 \quad (\text{calculated, Pait et al. 1992})
\]

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

\[
2.34 \quad (\text{calculated-S, Kenaga 1980})
\]
\[
2.23 \quad (\text{calculated-MCI \chi, Gerstl & Helling 1987})
\]
\[
2.33 \quad (\text{selected, Trevisan et al. 1991})
\]
\[
2.19 \quad (\text{Montgomery 1993})
\]
\[
2.17 \quad (\text{soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996})
\]
\[
2.38–2.90 \quad (\text{Tomlin 1994})
\]

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

**Volatilization:**

- Photolysis: \( t_{1/2} = 34 \text{ d for 82\% of 200\, \mu g/mL to degrade in distilled water under sunlight (Moilnen & Crosby 1972; quoted, Cessna & Grover 1991);} \)
- \( t_{1/2} = 2.25 \text{ h for 37–51\% of 100\, \mu g mL}^{-1} \text{ to degrade in distilled water under > 300 nm light (Tanaka et al. 1981; quoted, Cessna & Grover 1991);} \)
- \( t_{1/2} = 245 \text{ h for 14–81\% of 15\, \mu g mL}^{-1} \text{ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Grover 1991);} \)
- Photolysis \( t_{1/2} = 12–13 \text{ h in water (Tomlin 1994).} \)

**Oxidation:** measured rate constant for reaction with hydroxyl radical, \( k(\text{aq.}) = 1.60 \times 10^{9} \text{ M}^{-1} \text{ s}^{-1} \text{ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).} \)

**Hydrolysis:** \( t_{1/2} > 4 \text{ months for 4360\, \mu g mL}^{-1} \text{ to hydrolyze in phosphate buffers pH 5–9 at 20°C (El-dib & Aly 1976; quoted, Muir 1991);} \)

\( t_{1/2} >> 1 \text{ yr at pH 4, 7, 9 at 22°C (Tomlin 1994).} \)
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Biodegradation: $t_{1/2} = 1–2$ d for 30 $\mu$g mL$^{-1}$ to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);

$t_{1/2} \sim 10$ d for 40 $\mu$g mL$^{-1}$ to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation: second-order microbial degradation rate constant $k = 5 \times 10^{-10}$ L-organisms$^{-1}$ h$^{-1}$ (Steen & Collette 1989).

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

Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{1/2} >> 1$ yr (pH 4, 7, 9) at 22°C and photolysis $t_{1/2} = 12–13$ h in aqueous solution (Tomlin 1994).

Groundwater: reported $t_{1/2} < 5$ d (Bottoni & Funari 1992)

Sediment: $t_{1/2} \sim 10$ d for 40 $\mu$g mL$^{-1}$ to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

Soil: $t_{1/2} = 1–2$ d for 30 $\mu$g mL$^{-1}$ to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);

selected field $t_{1/2} = 1.0$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996);

soil $t_{1/2} = 15$ d (Pait et al. 1992);

$\sim 5$ d (Bottoni & Funari 1992).

Biota:
17.1.1.69 Propazine

Common Name: Propazine
Synonym: G-30028, Geigy 30028, Gesamil, Maax, Milogard, Plantulin, Primatol P, Propasin, Prozinex
Chemical Name: 6-chloro-\(N,N'\)-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine
Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in milo and sweet sorghum.
CAS Registry No: 139-40-2
Molecular Formula: \(C_9H_{16}ClN_5\)
Molecular Weight: 229.710
Melting Point (°C): 213 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
272.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
1.85 (\(pK_a\), Weber 1970; quoted, Bintein & Devillers 1994)
1.80 (\(pK_a\), Weber et al. 1980; Willis & McDowell 1982)
1.85 (\(pK_a\), Herbicide Handbook 1989)
1.70 (\(pK_a\), 21°C, Worthing & Hance 1991)
12.15 (\(pK_b\), Wauchope et al. 1992)
1.85 (\(pK_a\), 22°C, Montgomery 1993)
12.3 (\(pK_b\), 21°C, Tomlin 1994)
Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):
41.84 (DSC method, Plato 1972)
Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}}\) = 56 J/mol K), \(F\): 0.0143 (mp at 213°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
10 (Gysin 1962)
8.6 (20–22°C, Bailey & White 1965; Spencer 1973; Quellette & King 1977)
4.82, 4.60, 5.05 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
8.60 (Martin & Worthing 1977)
4.8–8.6 (Weber et al. 1980)
5.0 (20°C, Spencer 1982)
8.50 (20°C, Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.87 × 10⁻⁶ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
\[
\log (P/\text{mmHg}) = 11.911 - 4933/(T/K), \text{ temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)}
\]
3.90 × 10⁻⁶ (20°C, Quellette & King 1977)
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Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 1.00 × 10⁻⁴ (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
- 1.00 × 10⁻³ (20°C, calculated-P/C, Montgomery 1993)
- 1.04 × 10⁻³ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{OW}$:

- 2.89 (Kenaga & Goring 1980; Yoshioka et al. 1986)
- 2.94 (shake flask-GC or UV, Brown & Flagg 1981)
- 2.59 (RP-HPLC-k' correlation, Braumann et al. 1983)
- 2.93 (shake flask, Biagi et al. 1991)
- 2.91 (RP-HPLC-RT correlation, Finizio et al. 1991)
- 2.91, 2.94 (Montgomery 1993)
- 2.77 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.93 (recommended, Sangster 1993; Hansch et al. 1995)
- 2.89 (shake flask-UV, Liu & Qian 1995)
- 3.13 (Pomona-database, Müller & Kördel 1996)
- 2.77 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 2.26 (calculated-S, Kenaga 1980)
- 0.903 (calculated-K_{OC}, Kenaga 1980)

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

- 2.20 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
- 3.11 (soil, calculated-S per Kenaga & Goring 1980; Kenaga 1980)
- 2.56 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.78 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 2.34 (estimated as log $K_{OM}$, Magee 1991)
- 2.18 (soil, quoted, Bottoni & Funari 1992)
- 1.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
- 1.69–2.56 (Montgomery 1993)
- 2.44 (selected, Lohninger 1994)
- 1.90, 2.0 (Tomlin 1994)
- 2.57 (calculated-K_{OW}, Liu & Qian 1995)
- 2.40 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.94; 2.55 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.59, 1.93, 2.08, 1.95, 2.70 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.18, 2.148, 2.10, 1.98, 2.58 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.40; 2.43; 2.84 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.15, 2.17 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 3.2–7.4, average, Delle Site 2001)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization:
Photolysis: 1 ppb contaminated water in presence of TiO₂ and H₂O₂ completely photodegraded after 3.5 h by solar irradiation (Muszkat et al. 1992).

Oxidation:
Hydrolysis: calculated rate constant k = 9.70 × 10⁻⁶ s⁻¹ with t½ = 83 d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water:
Ground water: reported half-lives or persistence, t½ = 80–100 d (Bottoni & Funari 1992)

Sediment:
Soil: persistence of 18 months (Edwards 1973; quoted, Morrill et al. 1982);
persistence of 12 months in soil (Wauchope 1978);
t½ = 62 d and 127 d in a Hatzenbühl soil at pH 4.8 and Neuhofen soil at pH 6.5 respectively at 22°C under laboratory conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);
reported t½ = 80–100 d (Bottoni & Funari 1992);
selected field t½ = 135 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:
17.1.1.70 Propham

Common Name: Propham
Synonym: Agermin, Ban-Hoe, Beet-Kleen, Birgin, Chem-Hoe, Collavin, IFC, IFK, INPC, IPC
Chemical Name: carbanilate acid isopropyl ester; isopropyl carbanilate; isopropyl-N-phenyl carbamate; 1-methylethyl phenylcarbamate
Uses: pre-emergence and post-emergence herbicide to control annual grass weeds in peas, beans, sugar beet, lettuce, lucerne, clover, flax, sunflowers and lentils.
CAS Registry No: 122-42-9
Molecular Formula: C_{10}H_{13}NO_{2}
Molecular Weight: 179.2 16
Melting Point (°C):
90 (Lide 2003)
Boiling Point (°C):
> 150 (sublimes but decomposes, Montgomery 1993)
Density (g/cm³ at 20°C):
1.09 (Spencer 1982; Tomlin 1994; Hartley & Kidd 1987; Milne 1995)
Molar Volume (cm³/mol):
213.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
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: 0.230 (mp at 90°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
100 (Freed 1953)
250 (Nex & Sweezey 1954; Ashton & Crafts 1981)
22.5–32 (Bailey & White 1965)
250 (20°C, Spencer 1973, 1982)
250–254 (Weber et al. 1980)
127 (selected, Gerstl & Helling 1987)
250 (20°C, Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
sublimes (rm. temp., Herbicide Handbook 1989)
sublimes (rm. temp., Montgomery 1993; Tomlin 1994)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
2.60 (20 ± 2°C, shake flask-UV, Briggs 1981)
2.16 (selected, Dao et al. 1983; Gerstl & Helling 1987)
2.27 (shake flask, Mitsutake et al. 1986)
2.60 (recommended, Sangster 1993)
Bioconcentration Factor, log BCF:

1.43 (calculated-S, Kenaga 1980)
0.301 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.71 (Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.32 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.71 (20 ± 2°C, reported as log K_{OM}, Briggs 1981)
1.93 (calculated-MCI χ, Gerstl & Helling 1987)
1.71 (Montgomery 1993)
2.30 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: direct t_{1/2} = 254 d in clear water body near the surface for a mid-summer day at latitude 40° (Wolfe et al. 1978)
direct t_{1/2} = 254 d in distilled water assuming for a mid-summer day at latitude 40°; t_{1/2} = 2.25 h for 1% of 100 µg/ml to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: t_{1/2} > 4 months for 3550 µg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)
k(alkaline) = 7.6 × 10^{-6} M^{-1} s^{-1} at 27°C, k = 5.6 × 10^{-5} M^{-1} s^{-1} at 50°C, k = 2.6 × 10^{-4} M^{-1} s^{-1} at 70°C; with t_{1/2} > 1 × 10^4 d at pH 5, 7 and 9 (Wolfe et al. 1978)

Biodegradation: t_{1/2} = 190 d by 1 mg/L fungus Asperillus fumigatus, t_{1/2} = 3.2 d by bacteria (Wolfe et al. 1978)
k = 1.5 × 10^{-2} L (mg M)^{-1} h^{-1} with t_{1/2} = 190 d for 2–25 µg/mL fungus Aspergillus fumigatus; k = 9 × 10^{-2} L (mg M)^{-1} h^{-1} with t_{1/2} = 3.2 d for bacteria Pseudomonas striata to biodegrade in stream water at pH 7 and 28°C (Muir 1991)
t_{1/2} ~ 30–40 d for 1–0.0004 µg/mL to biodegrade in filtered sewage water at 20–22°C and t_{1/2} ~ 20 to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991)
t_{1/2}(aerobic) > 4 months for 6–7 µg/mL to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: hydrolysis t_{1/2} > 1 × 10^4 d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis t_{1/2} = 254 d assuming a mid-summer day at altitude 40°, and biolysis t_{1/2} = 190 d for 1 mg/L of fungus and t_{1/2} = 3.2 d for bacteria at 28°C (Wolfe et al. 1978);
t_{1/2} ~ 30–40 d for 1–0.0004 µg/mL to biodegrade in filtered sewage water at 20–22°C and t_{1/2} ~ 20 to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991);
aerobic t_{1/2} > 4 months for 6–7 µg/mL to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Ground water:

Sediment:

Selected field: t_{1/2} = 15 d in soil and t_{1/2} = 5 d at 16 and 29°C (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);
selected field t_{1/2} = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:
17.1.1.71 Pyrazon

Common Name: Pyrazon
Synonym: chloridazon, chloridazone, Blurex, Burex, Dazon, Phenosane, Piramin, Pyramin
Chemical Name: 5-amino-4-chloro-2-phenylpyridazin-3(2H)-one
Uses: as pre- and post-emergence herbicide to control of annual broadleaf weeds in sugar-beet, fodder beet and beet root; and also used in combination with other herbicides, etc.
CAS Registry No: 1698-60-8
Molecular Formula: \( \text{C}_{10}\text{H}_8\text{ClN}_3\text{O} \)
Molecular Weight: 221.643
Melting Point (°C): 205 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
2.14 (Tomlin 1994)
Molar Volume (cm³/mol):
205.7 (calculated-Le Bas method at normal boiling point)
143.9 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
26.59 (DSC method, Plato & Glasgow 1969)
Entergy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 0.0171 (mp at 205°C)
0.013 (20°C, Suntio et al. 1988)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
300 (20°C, Khan 1980)
400 (20°C, Spencer 1982)
360 (20°C, selected, Suntio et al. 1988)
340 (20°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
9.86 (40°C, Ashton & Craft 1973; Spencer 1982)
< 0.00001 (20°C, Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)
7.0 (20°C, estimated, Suntio et al. 1988)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
4.31 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
1.50 (selected, Gerstl & Helling 1987)
1.12 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.19 (pH 7, Tomlin 1994)
Bioconcentration Factor, log BCF:
  1.32 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log $K_{OC}$:
  2.12, 2.18 (selected, calculated-MCI $\chi$, Gerstl & Helling 1987)
  2.74 (soil, calculated-MCI and fragments contribution method, Meylan et al. 1992)
  2.08 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
  1.95–2.53 (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives:
  Photolysis: $t_{1/2} = 150$ h at pH 7 in simulated sunlight and $t_{1/2} = 47.7$ h by 80000 lux, xenon lamp (Tomlin 1994).

Half-Lives in the Environment:
  Soil: field $t_{1/2} = 21$ d (Wauchope et al. 1992; Hornsby et al. 1996)
17.1.1.72 Simazine

Common Name: Simazine
Chemical Name: 6-chloro-N,N′-diethyl-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(ethyl-amino)-1,3,5-triazine
Uses: selective pre-emergence systemic herbicide to control many broadleaf weeds and annual grasses in deep-rooted fruit and vegetable crops.
CAS Registry No: 122-34-9
Molecular Formula: C₇H₁₂ClN₅
Molecular Weight: 201.657
Melting Point (°C): 226 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.302 (Hartley & Kidd 1987; Milne 1995)
1.203 (Montgomery 1993)
Molar Volume (cm³/mol):
228.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
1.65 (pKₐ, Weber 1970; quoted, Binten & Devillers 1994)
1.60 (pKₐ, Weber et al. 1980; Willis & McDowell 1982)
1.70 (pKₐ, 21°C, Worthing & Hance 1991; Montgomery 1993)
2.00 (pKₐ, Yao & Haag 1991; Haag & Yao 1992)
12.3 (pKₑₐ, Tomlin 1994)
Enthalpy of Fusion, ΔHₓₛ (kJ/mol):
43.932 (DSC method, Plato 1972)
Entropy of Fusion, ΔSₓₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₓₛ = 56 J/mol K), F: 0.0107 (mp at 226°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
5.0 (Bailey & White 1965 Freed 1976; Wauchope 1978)
5.8, 5.0, 5.0 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
15.1 (26°C, Getzen & Ward 1971)
5.0 (20°C, Weber 1972; Spencer 1973; Khan 1980)
5.0 (20°C, Martin & Worthing 1977; Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)
5.0, 3.50, 7.4(20°C, quoted, exptl., calculated-Parachor & mp, Briggs 1981)
3.5–5.0 (20°C), Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
8.13 × 10⁻⁷ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)

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2.00 × 10⁻⁶ (gas saturation, Spencer & Cliath 1974)
8.00 × 10⁻⁷ (20–25°C, Weber et al. 1980; Willis & McDowell 1982)
8.50 × 10⁻⁶ (20°C, selected, Suntio et al. 1988)
4.80 × 10⁻⁶ (30°C, Suntio et al. 1988)
2.94 × 10⁻⁶ (OECD 104, Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
3.40 × 10⁻⁴ (20°C, calculated-P/C, Suntio et al. 1988)
8.40 × 10⁻⁵ (calculated-P/C, Taylor & Glotfelty 1988)
3.30 × 10⁻⁵ (20°C, calculated-P/C, Muir 1991)
3.40 × 10⁻⁴ (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.19 (Kenaga & Goring 1980)
1.94 (Rao & Davidson 1980)
1.51 (shake flask-UV, Lord et al. 1980)
1.51 (20 ± 2°C, shake flask-UV, Briggs 1981)
2.16 (shake flask, Brown & Flagg 1981)
1.96, 2.06 (RP-HPLC-k’ correlation, McDuffie et al. 1981)
2.27 (selected, Dao et al. 1983; Gerstl & Helling 1987)
2.14 (shake flask, Mitsutake et al. 1986)
1.50 (Nicholls 1988)
2.18 (shake flask, Biagi et al. 1991)
2.26, 2.20 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
1.96 (Worthing & Hance 1991; Milne 1995)
2.00 (shake flask, pH 7, Baker et al. 1992)
1.94–2.26 (Montgomery 1993)
2.07 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.18 (recommended, Sangster 1993)
2.10 (Tomlin 1994)
2.18 (shake flask-UV, Liu & Qian 1995)
2.18 (recommended, Hansch et al. 1995)
2.51 (Pomona-database, Müller & Kördel 1996)
2.07 (RP-HPLC-RT correlation, Finizio et al. 1997)
1.83 (RP-HPLC-RT correlation, Nakamura et al. 2001)
1.49 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
2.48 (calculated-S, Kenaga 1980)
0.778 (calculated-K_{OC}, Kenaga 1980)
2.16 (earthworms, Lord et al. 1980)
0.699 (calculated-K_{OC}, Briggs 1981)

Sorption Partition Coefficient, log K_{OC}:
2.13 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980)
3.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.15 (av. soils/sediments, Rao & Davidson 1980)
1.68 (20 ± 2°C, K_{OM} multiplied by 1.724, Briggs 1981)
2.33 (Georgia’s Hickory Hill pond sediment, Brown & Flagg 1981)
3.66, 2.53, 1.77 (estimated-S, calculated-S and mp, estimated-K_{OC}, Karickhoff 1981)
2.14 (soil average, Jury et al. 1983)
Herbicides

2.20, 2.15 (selected, calculated-MCI $\chi$, Gerstl & Helling 1987)
2.15 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
1.60–2.20 (Carsel 1989)
1.92 (estimated as log $K_{OM}$, Magee 1991)
2.13–3.34, 2.15, 2.45, 2.70 (soil, quoted values, Bottoni & Funari 1992)
3.02 (average of 12 soils, calculated-linearize Freundlich Isotherm, Sukop & Cogger 1992)
2.14 (Montgomery 1993)
1.78 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.37 (selected, Lohninger 1994)
2.01–2.58 (Tomlin 1994)
2.18 (calculated-$K_{ow}$, Liu & Qian 1995)
2.10 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
1.79; 2.17 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.07, 1.65, 1.68, 1.61, 2.48 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.625, 1.90, 1.69, 1.66, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.625, 1.901, 1.689, 1.656, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-$k^{‘}$ correlation, Gawlik et al. 2000)
2.10; 2.10, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.29, 2.29, 2.29 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, pH 3.2–8.0, average, Delle Site 2001)
2.50, 2.34, 2.10 (soils with organic carbon OC $\geq$ 0.5% at: pH 3.2–5.0, pH 5.1–5.9, pH $\geq$ 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatileization: $t_{1/2} = 276$ d (Jury et al. 1983; quoted, Grover 1991); measured rate constant $k = 600$ d$^{-1}$ and estimated rate constant $k = 1000$ d$^{-1}$ (Glotfelty et al. 1989).
Photolysis:
Oxidation:
\[ k(aq.) = 5.9 \times 10^9 \text{ M}^{-1} \text{s}^{-1} \text{ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and 24 \pm 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992).} \]
\[ k(aq.) = (4.8 \pm 0.2) \text{ M}^{-1} \text{s}^{-1} \text{ for direct reaction with ozone in water at pH 4.3 and 23°C, with } t_{1/2} = 1.9 \text{ h at pH 7 (Yao & Haag 1991).} \]
\[ k(aq.) = (2.8 \pm 0.2) \times 10^9 \text{ M}^{-1} \text{s}^{-1} \text{ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and 24 \pm 1°C (Haag & Yao 1992).} \]
Hydrolysis: calculated rate constant $k = 8.32 \times 10^{-6}$ s$^{-1}$ with $t_{1/2} = 96$ d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).
Biodegradation: rate constant $k = 0.014$ d$^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
$\text{t}_{1/2} = 8–27$ d for 3 $\mu$g mL$^{-1}$ to biodegrade in pond sediment/water and $\text{t}_{1/2} > 32$ d in pond water both at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);
$\text{t}_{1/2} = 75$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);
microbial degradation $\text{t}_{1/2} = 70–11$ d in soil (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $\text{t}_{1/2} > 32$ d for 3 $\mu$g mL$^{-1}$ to biodegrade in pond water at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);
$\text{t}_{1/2} = 1–4$ wk in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);
$t_{1/2} \sim 30$ d in ponds (Herbicide Handbook 1989);
measured rate constant $k = (4.8 \pm 0.2) \text{ M}^{-1} \text{s}^{-1}$ for direct reaction with ozone in water at pH 4.3 and 23°C,
with $t_{1/2} = 1.9$ h at pH 7 (Yao & Haag 1991).

Ground water: reported half-lives or persistence, $t_{1/2} = 15–75$, 46–174 and 56 d (Bottoni & Funari 1992)
Sediment: $t_{1/2} = 8–27$ d for 3 μg mL$^{-1}$ to biodegrade in pond sediment/water at 25°C (Tucker & Boyd 1981;

Soil: estimated persistence of 12 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
persistence of 12 months (Wauchope 1978);
estimated first-order $t_{1/2} = 49.5$ d from biodegradation rate constant $k = 0.014$ d$^{-1}$ by soil incubation die-away
studies (Rao & Davidson 1980; quoted, Scow 1982);
$t_{1/2} = 45$ d in Hatzenbühl soil at pH 4.8 and $t_{1/2} = 100$ d in Neuhofen soil at pH 6.5 both at 22°C, respectively,
under lab. conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);
$t_{1/2} = 1–6$ months (Jones et al. 1982; quoted, Meakins et al. 1994);
$t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
moderately persistent in soils with $t_{1/2} = 20–100$ d (Willis & McDowell 1982);
degradation rate constant $k = (1.51 \pm 0.086) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 45.9$ d in control soil and $k = (1.76 \pm 0.177) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 73.5$ d in
control soil and $k = (0.864 \pm 0.048) \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 80.2$ d in pretreated soil once only in the
laboratory (Walker & Welch 1991);
reported $t_{1/2} = 15–75$, 46–174 and 56 d; 29 d at 5°C and $t_{1/2} = 209$ d at 30°C (Bottoni & Funari 1992);
selected field $t_{1/2} = 60$ d (Wauchope et al. 1991, 1992; quoted, Dowd et al. 1993; Richards & Baker 1993;
quoted, Halfon et al. 1996; Hornsby et al. 1996);
soil $t_{1/2} = 75$ d (Pait et al. 1992);
degradation by microorganism in biometer systems: $t_{1/2} = 58$ d in silty sand standard laboratory conditions,
$t_{1/2} = 87$ d for corrected standard conditions and $t_{1/2} = 91$ d in simulated outdoor conditions; $t_{1/2} = 51$ d in
silty loam standard laboratory conditions, $t_{1/2} = 77$ d corrected standard conditions, $t_{1/2} = 63$ d in simulated
outdoor conditions at constant soil moisture and 20°C. Degradation by microorganism in outdoor experi-
ments in small lysimeter systems: $t_{1/2} = 32$ d outdoor fallow, $t_{1/2} = 35$ d outdoor barley in silty sand, and
$t_{1/2} = 49$ d outdoor fallow, $t_{1/2} = 53$ d outdoor barley in silty loam (Rüdel et al. 1993)
t$= 49–50$ d in 0–40 cm soil cores taken from: cultivated field; from meadow $t_{1/2} = 32–39$ d and from gravel
track $t_{1/2} = 62–51$ d (Hassink et al. 1994);
degradation $t_{1/2} = 70–110$ d (Tomlin 1994).

Biota: biochemical $t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

![Graph](image_url)

**FIGURE 17.1.1.72.1** Logarithm of vapor pressure versus reciprocal temperature for simazine.

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17.1.1.73 2,4,5-T

Common Name: 2,4,5-T
Chemical Name: 2,4,5-trichlorophenoxyacetic acid
Uses: herbicide to control undesirable brush and woody plants; also used as plant hormone, defoliant.
CAS Registry No: 93-76-5
Molecular Formula: C₈H₅Cl₃O₃
Molecular Weight: 255.483
Melting Point (°C):
153 (Lide 2003)
Boiling Point (°C):
> 200 (dec., Howard 1991)
Density (g/cm³ at 20°C):
1.80 (25°C; Que Hee et al. 1981)
1.80 (Spencer 1982; Budavari 1989; Milne 1995)
Molar Volume (cm³/mol):
226.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
2.88 (potentiometric titration, Nelson & Faust 1969)
2.85 (Cessna & Grover 1978; Somasundaram et al. 1991; Augustijn-Beckers et al. 1994)
2.70 (Haag & Yao 1992)
2.80–2.88 (Montgomery 1993)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
107.8 (Rordorf 1989)
Enthalpy of Fusion, ΔH₈₅ (kJ/mol):
34.936 (DSC method, Plato & Glasgow 1969)
34.2 (Rordorf 1989)
Entropy of Fusion, ΔS₈₅ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₈₅ = 56 J/mol K), F: 0.0555 (mp at 153°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
268 (shake flask-UV, Leopold et al. 1960)
238 (20°C, Loos 1975)
238 (Martin & Worthing 1977)
238–280 (Weber et al. 1980)
278 (Spencer 1982; Verschueren 1983)
278 (20°C, Hartley & Kidd 1987)
280 (selected, Gerstl & Helling 1987)
150 (Worthing & Walker 1987, Worthing & Hance 1991)
220 (20°C, Montgomery 1993)
278 (20–25°C, selected, Augustijn-Beckers et al. 1994)
238 (20°C, Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.0063 (effusion method, Hamaker & Kerlinger 1971)
< 1.0 × 10⁻⁶ (20°C, Hartley & Kidd 1983)
0.005 (20°C, selected, Suntio et al. 1988; Riederer 1990)
< 1.0 × 10⁻³ (20°C, Hartley & Kidd 1983; 1987)
2.30 × 10⁻⁶, 1.90 × 10⁻⁴, 8.50 × 10⁻³, 0.230, 4.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 19.238 – 7418.9/(T/K); measured range 80.4–145°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 15.058 – 5632.4/(T/K); measured range 80.4–145°C (liquid, gas saturation-GC, Rordorf 1989)
7.00 × 10⁻⁷ (Worthing & Hance 1991)
0.0040 (20°C, Montgomery 1993)
0.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
8.79 × 10⁻⁴ (Hine & Mookerjee 1975)
0.0058 (20°C, calculated-P/C, Suntio et al. 1988)
0.0049 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K OW:
3.13 (electrometric titration, Freese et al. 1979)
0.60 (pH dependent quoted from Dow Chemical data, Kenaga & Goring 1980)
0.85 (Rao & Davidson 1980)
2.99 (RP-HPLC-k’ correlation, Braumann et al. 1983)
3.13 (Hansch & Leo 1985)
3.40 (OECD 81 method, Kerler & Schönherr 1988)
3.36 (selected, Travis & Arms 1988)
3.31 (shake flask-HPLC/UV, Jafvert et al. 1990)
0.60–3.40 (Montgomery 1993)
3.13 (countercurrent LC, Ilchmann et al. 1993)
3.13 (selected, Sangster 1993)
3.13 (recommended, Hansch et al. 1995)
3.31 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log B CF:
−4.55 (milk biotransfer factor log B m, correlated-K OW, Bjerke et al. 1972)
1.18 (measured, Isensee 1976)
−4.82 (beef biotransfer factor log B b, correlated-K OW, Kenaga 1980)
1.63 (fish under flowing water conditions, Kenaga & Goring 1980)
1.45 (calculated-S, Kenaga 1980)
0.301 (calculated-K OC, Kenaga 1980)
1.36–1.40 (fish under static ecosystem tests, Kenaga & Goring 1980; Garten & Tralbalka 1983)
1.41 (mosquito fish 32 d under unspecified conditions, Ang et al. 1989)

Sorption Partition Coefficient, log K OC:
1.72 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.93, 2.27, 2.31, 2.31, 2.45, 2.31 (sand soil, whole soil, fine soil, coarse clay soil, medium silt soil, coarse silt soil, Nkedi-Kizza et al. 1983)
2.38 (calculated-MCI χ, Gerstl & Helling 1987)
1.90 (soil, screening model calculations, Jury 1987b)
1.72 (soil, Sabljic 1987)
1.77; 2.63; 1.94 (Alfisol soil, Podzol soil; sediment, von Oepen et al. 1991)
1.72, 2.27 (Montgomery 1993)
1.90 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)
Herbicides

1.72 (estimated-chemical structure, Lohninger 1994)
1.99 (soil, calculated-QSAR MCI \( \chi \), Sabljic et al. 1995)
1.99 (1.63–2.35) (soils: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

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

Volatilization:
Photolysis: \( t_{1/2} = 48 \) h for 17–80% of 1 \( \mu \)g/mL to degrade in buffered aqueous solution at pH 7.8 under sunlight (Crosby & Wong 1973; quoted, Cessna & Muir 1991);
\( t_{1/2} = 15 \) d for < 2.6 \( \mu \)g/mL to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);
\( t_{1/2} = 8.7 \) d for < 2.6 \( \mu \)g/mL to degrade in aqueous fulvic acid solution (17 mg/L) and \( t_{1/2} = 3.5 \) d for < 2.6 \( \mu \)g/mL to degrade in aqueous fulvic acid solution (55 mg/L) under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991).

Oxidation:
photooxidation \( t_{1/2} = 12.2–122 \) h in air, based on an estimated rate constant for the reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991)
\( k(aq.) = (8.9 \pm 1.3) \) M\(^{-1}\) s\(^{-1}\) for direct reaction with ozone in water at pH 1.7–5.0 and 26°C, with \( t_{1/2} = 1.0 \) h at pH 7 (Yao & Haag 1991)
\( k_{OH} \) (calc) = \( 4.0 \times 10^9 \) M\(^{-1}\) s\(^{-1}\) for reaction with hydroxyl radical in aqueous solutions (Haag & Yao 1992).

Hydrolysis: will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes (Kollig 1993).

Biodegradation:
\( t_{1/2} \) (aerobic) = 27 d for 50 \( \mu \)g/mL in sediment-water microcosm by long lag phase degradation (Alexander 1974; quoted, Muir 1991)
\( t_{1/2} \) (aerobic) = 240–480 h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991)
\( k = 0.001 \) d\(^{-1}\) by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)
\( k = 0.035 \) d\(^{-1}\) by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982)
\( k = 0.01–0.03 \) d\(^{-1}\) at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

\( t_{1/2} = 33 \) d from screening model calculations (Jury et al. 1987b)
\( t_{1/2} \) (anaerobic) = 672–4320 h, based on anaerobic digester sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Air: \( t_{1/2} = 12.2–122 \) h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: estimated first-order \( t_{1/2} = 693 \) d from biodegradation rate constant \( k = 0.001 \) d\(^{-1}\) by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)
\( t_{1/2} = 240–480 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

extremely resistant degradation in natural water with \( t_{1/2} = 580 \) d for static sediment-sea water to \( t_{1/2} = 1400 \) d for static estuarine river water (Muir 1991);
measured rate constant \( k = (8.9 \pm 1.3) \) M\(^{-1}\) s\(^{-1}\) for direct reaction with ozone in water at pH 1.7–5.0 and 21 ± 1°C, with \( t_{1/2} = 3.9 \) h at pH 7 (Yao & Haag 1991).

Ground water: \( t_{1/2} = 480–4320 \) h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).
Sediment: estimated first-order \( t_{1/2} = 23–69.3 \) d from biodegradation rate constant \( k = 0.01–0.03 \) d\(^{-1}\) at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)
\( t_{1/2} = 27 \) d for sediment-water microcosm under aerobic conditions (quoted, Muir 1991).
Soil: degradation \( t_{1/2} = 24 \) d and 14 d in Quachita Highlands’ forest and grassland soil, respectively, \( t_{1/2} = 21 \) d in Gross Timbers Forest soil, average \( t_{1/2} = 17 \) d in 3 soils (Altom & Stritzke 1973);
$t_{1/2} = 240-480 \text{ h}$, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991);
estimated first-order $t_{1/2} = 19.8 \text{ d}$ from rate constant $k = 0.035 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
$t_{1/2} = 33 \text{ d}$ from screening model calculations (Jury et al. 1987b);
aerobic degradation $t_{1/2} > 25 \text{ d}$ at $29^\circ \text{C}$, to $t_{1/2} = 58 \text{ d}$ at $21^\circ \text{C}$ in soil suspension from pre-incubated soil (Muir 1991);
selected field $t_{1/2} = 30 \text{ d}$ (Augustijn-Beckers et al. 1994).
Biota: biochemical $t_{1/2} = 33 \text{ d}$ from screening model calculations (Jury et al. 1987b).
17.1.1.74 Terbacil

Common Name: Terbacil
Synonym: Sinbar, Turbacil
Chemical Name: 3-\textit{tert}-butyl-5-chloro-6-methyluracil
CAS Registry No: 5902-51-2
Uses: control of most annual grasses and broadleaf weeds, and some perennial weeds in established apples, asparagus, blueberries, citrus, lucerne, mint, peaches, pecans, strawberries, and sugar cane, etc.
Molecular Formula: C₉H₁₃ClN₂O₂
Molecular Weight: 216.664
Melting Point (°C):
176 (Lide 2003)
Boiling Point (°C):
sublime(below mp, Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
217.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
9.0 (Wauchope et al. 1992)
Enthalpy of Fusion, ΔHₜₖₑₜ (kJ/mol):
Entropy of Fusion, ΔSₜₖₑₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₖₑₜ = 56 J/mol K), F: 0.0330 (mp at 176°C)
0.027 (20°C, Suntio et al. 1988)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
710 (Ashton & Crafts 1973; 1981; Spencer 1982)
710 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
600 (20°C, selected, Suntio et al. 1988)
Vapor Pressure (Pa at 25°C or as indicated):
6.40 × 10⁻⁵ (29.5°C, Ashton & Crafts 1973; 1981)
6.00 × 10⁻⁵ (30°C, Hartley & Kidd 1987)
5.00 × 10⁻⁵ (20°C, selected, Suntio et al. 1988)
6.00 × 10⁻⁵ (20°C, Montgomery 1993)
6.25 × 10⁻⁵ (29.5°C, Tomlin 1994)
1.91 × 10⁻³ (20–25°C, supercooled liquid value, quoted, Majewski & Capel 1995)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.80 × 10⁻⁵ (20°C, calculated-P/C, Suntio et al. 1988)
1.82 × 10⁻⁵ (20–25°C, calculated, Montgomery 1993)
1.53 × 10⁻³ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₜₘₜₚ:
1.89 (Karickhoff et al. 1979)
1.89 (Rao & Davidson 1980)
1.89, 1.90 (quoted, Montgomery 1993)
1.89  (recommended, Sangster 1993)
1.91  (Tomlin 1994)
1.89  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.18  (calculated-S, Kenaga 1980)
1.74  (Montgomery 1993)

Sorption Partition Coefficient, log $K_{OC}$:
1.71, 2.08  (soil: exptl., calculated, Kenaga 1980; Kenaga & Goring 1980)
1.62, 1.98  (soil, quoted, Madhun et al. 1986)
1.89, 1.76; 1.82, 1.04 (estimated-$K_{OW}$; solubilities, Madhun et al. 1986)
1.62  (soil, screening model calculations, Jury et al. 1987b)
1.74  (soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.32–2.20 (soil, quoted, Montgomery 1993)
1.66  (soil, calculated-QSAR MCI $\chi$, Sabljic et al. 1995)
1.58 (1.38–1.78) (soils: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Biodegradation: $t_{1/2} = 50$ d (Jury et al. 1987b).

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil: moderately persistent in soil with $t_{1/2} = 20–100$ d (Willis & McDowell 1982);
$t_{1/2} \sim 5–7$ months (Hartley & Kidd 1987);
$t_{1/2} = 50$ d from screening model calculations (Jury et al. 1987b);
field $t_{1/2} = 50–175$ d and the selected $t_{1/2} = 120$ d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota: biochemical $t_{1/2} = 50$ d (Jury et al. 1987b).
17.1.1.75 Terbutryn

Common Name: Terbutryn
Synonym: Clarosan, GS 14260, Igran, Prebane, Shortstop, Terbutrex, Terbutrin, Terbutryn
Chemical Name: N-(1,1-dimethylethyl)-N′-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2-(tert-butylamino)-4-(ethylamino)-6-(methylthio)-s-triazine
Uses: selective herbicide to control annual broadleaf and grass weeds in wheat.
CAS Registry No: 886-50-0
Molecular Formula: C_{10}H_{19}N_{5}S
Molecular Weight: 241.357
Boiling Point (°C): 154–160 (at 0.06 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Density (g/cm³ at 20°C): 1.115 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Molar Volume (cm³/mol): 273.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
   4.30 (pK_a, Worthing & Hance 1991)
   4.07 (pK_b, Montgomery 1993)
Enthalpy of Vaporization, ΔH_v (kJ/mol): 101.4 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 22.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K): 59 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{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):
   58 (20°C, Quellette & King 1977)
   25 (shake flask-HPLC, Ellgehausen et al. 1981)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   0.00013 (20°C, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991)
   0.00013 (20°C, Ashton & Crafts 1973; 1981)
   0.00013 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)
2.20 × 10⁻⁴, 9.10 × 10⁻³, 0.22, 3.40, 38.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_v/Pa) = 17.151 – 6201.4/(T/K); measured range 45–100°C (solid, gas saturation-GC, Rordorf 1989)
log (P_v/Pa) = 14.654 – 5297.1/(T/K); measured range 109–139°C (liquid, gas saturation-GC, Rordorf 1989)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

0.0013 (20°C, calculated-P/C, Suntio et al. 1988)
0.0012 (20°C, calculated-P/C, Muir 1991)
0.0120 (20°C, calculated-P/C, Montgomery 1993)
0.0014 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{OW}$:

3.74 (shake flask-GC, Elkell & Walum 1979)
3.72, 3.74 (shake flask, Ellgehausen et al. 1981)
2.56 (RP-HPLC-$k'$ correlation, Braumann et al. 1983)
3.34 (Worthing & Walker 1987)
3.43 (RP-HPLC-RT correlation, Finizio et al. 1991)
3.49 (Worthing & Hance 1991; Milne 1995)
3.43–3.73 (Montgomery 1993)
3.34 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.74 (recommended, Sangster 1993)
3.44 (Pomona-database, Müller & Kördel 1996)
3.34 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log $BCF$:

1.17 ($Daphnia magna$, wet wt. basis, Ellgehausen et al. 1980)
2.00, 2.00 (calculated-S, calculated-$K_{OC}$, Kenaga 1980)
1.95 (catfish $Ictalurus melas$, wet wt basis, Wang et al. 1996)

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

2.85 (soil, Colbert et al. 1975; Gaillardon et al. 1977, Kenaga 1980; Kenaga & Goring 1980)
2.87 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.85–2.87 (soil, quoted values, Bottoni & Funari 1992)
2.68 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
3.21–4.07 (Montgomery 1993)
3.30 (estimated-chemical structure, Lohninger 1994)
2.84 (calculated-$K_{OC}$, Liu & Qian 1995)
2.85 (soil, calculated-MCI 1,$\chi$, Sabljic et al. 1995)
2.68; 2.80 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.85; 2.82, 2.74 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.79 (3.28–4.30) (soil: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)
2.59, 2.86 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

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

Volatilization:
Photolysis: 4 ppb contaminated water in the presence of TiO$_2$ and H$_2$O$_2$ completely photodegraded after 15 h by solar irradiation (Muszkat et al. 1992).

Oxidation:
Hydrolysis:
Biodegradation: aerobic $t_{1/2} = 80–240$ d for $1 \mu g/mL$ to biodegrade in sediment-water and anaerobic $t_{1/2} > 650$ d for $1 \mu g/mL$ to biodegrade in sediment-water both at $25^\circ C$ (Muir & Yarechewski 1982; quoted, Muir 1991). Biological degradation rate followed a first order kinetics, with $t_{1/2} = 8.9–18.2$ d by raw water microflora from Rivere Nile, $t_{1/2} = 4.0–6.9$ d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

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

$k_1 = 1.70$ h$^{-1}$ (Chironomus tentans larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 1.9–1.5$ h$^{-1}$ (Chironomus tentans larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6–2.7$ h$^{-1}$ (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6–4.4$ h$^{-1}$ (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_1 = 0.053$ h$^{-1}$ (Chironomus tentans larvae in pond sediment-water system, calculated by initial uptake data of 0–12 h, Muir et al. 1983)

$k_1 = 0.043$ h$^{-1}$ (Chironomus tentans larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

$k_1 = 0.040$ h$^{-1}$ (Chironomus tentans larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_1 = 0.040$ h$^{-1}$ (Chironomus tentans larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 3.11$ h$^{-1}$, $k_2 = 0.0346$ h$^{-1}$ (catfish Ictalurus melas, Wang et al. 1996)

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} = 8.9–18.2$ d by raw water microflora from River Nile, $t_{1/2} = 4.0–6.9$ d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water: reported half-lives or persistence, $t_{1/2} = 14–28$ d (Bottoni & Funari 1992)

Sediment: aerobic $t_{1/2} = 80–240$ d for $1 \mu g mL^{-1}$ to biodegrade in sediment-water and anaerobic $t_{1/2} > 650$ d for $1 \mu g mL^{-1}$ to biodegrade in sediment-water both at $25^\circ C$ (Muir & Yarechewski 1982; quoted, Muir 1991). Soil: reported $t_{1/2} = 14–28$ d (Worthing & Hance 1991; Bottoni & Funari 1992); $t_{1/2} = 42$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $t_{1/2} = 13.1$ h in pond sediment-water, $t_{1/2} = 16.1$ h in river water, $t_{1/2} = 17.3$ h in river sediment-water, $t_{1/2} = 17.3$ in sand-water systems (Chironomus tentans larvae, Muir et al. 1983)
17.1.1.76 Thiobencarb

Common Name: Thiobencarb
Synonym: bentiocarb, Bolero, Saturn, Saturno, Siacarb
Chemical Name: \( S-(4\text{-chlorophenyl})\text{methyl diethylcarbamothioate} \)
Pesticide Class: herbicide; Group: carbamate
Uses: herbicide
CAS Registry No: 28249-77-6
Molecular Formula: \( \text{C}_{12}\text{H}_{16}\text{ClNOS} \)
Molecular Weight: 257.779
Melting Point (°C):
- 1.7 (Lide 2003)
Boiling Point (°C):
- 126–129/0.008 mmHg (Ashton & Crafts 1981)
- 126–128/0.008 mmHg (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant \( pK_a \):
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 30 (Ashton & Crafts 1981)
- 30 (reported as 30 g/L, Spencer 1982)
- 17.0 (Majewski & Capel 1995)
Vapor Pressure (Pa at 25°C or as indicated):
- \( 1.96 \times 10^{-4} \) (20°C, Ashton & Crafts 1981)
- \( 4.21 \times 10^{-3} \) (20°C, GC-RT correlation, Kim 1985)
- \( 2.0 \times 10^{-4} \) (20°C, Hartley & Kidd 1987)
- \( 1.97 \times 10^{-4} \) (Herbicide Handbook 1989)
- \( 2.93 \times 10^{-3} \) (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- \( 1.78 \times 10^{-3} \) (Majewski & Capel 1995)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.027 (calculated-P/C, Majewski & Capel 1995)
- 0.0274 (quoted lit., Armbrust 2000)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
- 3.42 (20°C, shake flask-GC, Kanazawa 1981)
- 3.40 (shake flask-GC, Schimmel et al. 1983)
- 3.98 (HPLC-RT correlation, Kawamoto & Urano 1989)
- 3.42 (Gerstl 1990)
3.40 (recommended, Sangster 1993)
3.93 (HPLC-RT correlation, Scibaldi & Finizio 1993)
3.40 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
3.78 (RP-HPLC-RT correlation, Yu et al. 1997)
4.37 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF or log $K_B$:

- 2.97 (Pait et al. 1992)
- 1.76, 1.77 (37.2, 18.6 µg/L concn in water; carp, 3–5 d exposure, Wang et al. 1992)
- 1.38, 1.0 (20.0, 2.0 µg/L concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
- 1.49, 1.13 (20.0, 2.0 µg/L concn in water; loach, 3–5 d exposure, Wang et al. 1992)
- 0.92, 1.08 (15.0, 7.5 µg/L concn in water; Grass carp, 3–5 d exposure, Wang et al. 1992)
- 1.20, 1.26 (10.0, 5.0 µg/L concn in water; eel, 3–5 d exposure, Wang et al. 1992)
- 2.57, 1.94 (5.0, 1.4 µg/L concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
- 0.46, 0.86 (200, 20 µg/L concn in water; freshwater clam, 3v5 d exposure, Wang et al. 1992)
- 1.82; 2.23 (Gnathopogon aerulescens; Pseudorasbora parva, flow-through condition, quoted, Devillers et al. 1996)

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

- 2.83 (soil, Gerstl 1990)
- 2.49, 3.02, 2.83 (soil, Bottini & Funari 1992)
- 2.95 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.43 (soil, calculated-χ, Meylan et al. 1992)
- 3.27 (calculated-QSAR MCI χ, Sabljic et al. 1995)
- 2.95 (quoted lit., Armbrust 2000)
- 3.32, 2.75 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis: stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 6.8 \times 10^{12}$ M$^{-1}$/h (Armbrust 2000)
- Biodegradation: $t_\frac{1}{2} = 2–3$ wk in soil varies under aerobic conditions to $t_\frac{1}{2} = 6–8$ months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)
  - aerobic degradation rate constant $k = 0.057$ d$^{-1}$ with $t_\frac{1}{2} = 12$ d by aerobic activated sludge at 20°C (Kawamoto & Urano 1990)
  - aerobic rate constant, $k = 1.38 \times 10^{-3}$ h$^{-1}$ (Armbrust 2000).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: Surface water: lost from aqueous solution by volatility and photodegradation (Herbicide Handbook 1989)
- biodegradation $t_\frac{1}{2} = 12$ d by aerobic activated sludge at 20°C (Kawamoto & Urano 1990).
- Ground water: reported half-lives or persistence, $t_\frac{1}{2} = 6–7$, 23–120, and 26–40 d (Bottoni & Funari 1992)
- Sediment:
- Soil: laboratory studies with Stockton adobe and Crowley silty clay loam gave $t_\frac{1}{2} = 2–3$ wk under aerobic conditions to $t_\frac{1}{2} = 6–8$ months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989);
  - reported half-lives or persistence of 6–7 d, 23–120 d, 26–40 d (Bottoni & Funari 1992);
- soil; $t_\frac{1}{2} = 18$ d (Pait et al. 1992); field $t_\frac{1}{2} = 21$ d (Wauchope et al. 1992; Hornsby et al. 1996).
- Biota:
17.1.1.77 Triallate

Common Name: Triallate
Synonym: Avadex BW, Buckle, CP 23426, Diphathal, Far-Go
Chemical Name: 2,3,3-trichloro-2-propene-1-thiol diisopropylcarbamate; \( S-(2,3,3\text{-trichloro-allyl})\text{diisopropyl-} \) (thio-carbamate); \( S-(2,3,3\text{-trichloro-2-propenyl}) \) bis(1-methylethyl)-carbamothioate

Uses: herbicide to control wild oats in lentils, barley, peas, and winter wheat.

CAS Registry No: 2303-17-5

Molecular Formula: \( C_{10}H_{16}Cl_{3}NOS \)
Molecular Weight: 304.664

Melting Point (°C):
- 29
  (Lide 2003)

Boiling Point (°C):
- 148–149
  (Khan 1980; Spencer 1982)
- 117
  (at 40 mPa, Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

Density (g/cm³ at 20°C):
- 1.273

Molar Volume (cm³/mol):
- 314.0
  (calculated-Le Bas method at normal boiling point)

Dissociation Constant \( pK_a \):

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
- 85.86
  (Rordorf 1989)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
- 27.7
  (Rordorf 1989)

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

Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \), \( F: 0.914 \) (mp at 29°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 4.0
  (20°C, Weber 1972; Weber et al. 1980)
- 4.0
- 4.0
- 4.0
- < 1.0
  (27°C, Ashton & Crafts 1981)
- 3.0
  (20°C, selected, Suntio et al. 1988)
- 4.0

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):
- 0.016
  (20°C, Weber 1972; Worthing & Walker 1987)
- 0.016
  (Ashton & Crafts 1973; Spencer 1982; quoted, Suntio et al. 1988)
- 0.0276
  (gas saturation-GC, measured range 20–45°C, Grover et al. 1978)
- 0.0265
  (29.5°C, Ashton & Crafts 1981)
- 0.0276
  (gas saturation method, Spencer & Cliath 1983)
- 6.07 \times 10^{-3}, 4.81 \times 10^{-3} (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
- 0.016
  (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 0.010
  (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
Herbicides 3665

0.015 (Herbicide Handbook 1989)
0.017* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
log (P/Pa) = 18.124 − 5932/(T/K); measured range 32.3–150°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 13.395 − 4485.1/(T/K); measured range 32.3–150°C (liquid, gas saturation-GC, Rordorf 1989)
0.026 (selected, Taylor & Spencer 1990)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.016 (20°C, Montgomery 1993)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.02 (20°C, calculated-P/C, Suntio et al. 1988)
1.983 (calculated-P/C, Taylor & Glotfelty 1988)
1.226 (20°C, calculated-P/C, Muir 1991)
0.762 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log Kₐₗₕ:
4.29 (Montgomery 1993)
4.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
2.45 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.18 (calculated-Kₒₛ, Kenaga 1980)

Sorption Partition Coefficient, log Kₒₛ:
3.56 (Guenzi & Beard 1974)
3.34 (soil, Grover 1974; Beestman & Demming 1976)
3.32 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
3.56 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
3.22 (soil, calculated-MCI ¹χ and fragments contribution, Meylan et al. 1992)
3.31 (calculated, Montgomery 1993)
3.38 (selected, Lohninger 1994)
3.35 (soil, calculated-MCI ¹χ, Sabljic et al. 1995)
3.60, 3.12 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.70, 2.64 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, tₜ:
Volatilization: tₜ = 26 d (Jury et al. 1983; quoted, Grover 1991); half-life of 100 d (Jury et al. 1984; quoted, Spencer & Cliaht 1990);
estimated tₜ ~ 8 d from 1 m depth of water at 20°C (Muir 1991).
Photolysis:
Hydrolysis: tₜ > 24 wk for 1 µg/mL to hydrolyze in aqueous buffer at pH 4, 7, and 9 in the dark at 25°C (Smith 1969; quoted, Muir 1991).
Biodegradation: estimated tₜ = 680 d at pH 6.8 and tₜ = 1170 d at pH 7.0, both at 25°C from biodegradation rate constants in aquatic systems (Smith 1969; quoted, Scow 1982);

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
Half-Lives in the Environment:


Surface water: \( t_{1/2} = 680 \text{ d at pH 6.8 and } t_{1/2} = 1170 \text{ d at pH 7.0, both at 25°C for biodegradation in aquatic systems (Smith 1969; quoted, Scow 1982).}

Ground water:

Sediment:

Soil: biodegradation \( t_{1/2} = 100 \text{ d from screening model calculations (Jury et al. 1984, 1987a,b; 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993); selected field } t_{1/2} = 82 \text{ d (Wauchope et al. 1992; Hornsby et al. 1996).}

Biota: biochemical \( t_{1/2} = 100 \text{ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).}

### TABLE 17.1.1.77.1

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

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( \log P = A - B/(T/K) )</th>
<th>( \ln P = A - B/(T/K) )</th>
<th>( \log P = A - B/(C + t/°C) )</th>
<th>( \ln P = A - B/(C + t/°C) )</th>
<th>( \log P = A - B/(T/K) - C\cdot\log (T/K) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.0133</td>
<td>18.124</td>
<td>5932</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0202</td>
<td>11.045</td>
<td>4401</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.0276</td>
<td>13.395</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>30</td>
<td>0.0446</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>45</td>
<td>0.267</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( A = 11.045 \text{ for liquid} \)

\( B = 4401 \text{ mmHg} \)

\( \text{eq. 1} \)

\( \text{eq. 1} \)

\( \text{eq. 1} \)

\( \text{eq. 1} \)

\( \text{eq. 1} \)

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( P/mmHg )</th>
<th>( \text{eq. 1} )</th>
<th>( A )</th>
<th>( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>33–33.5°C</td>
<td>18.124</td>
<td>5932</td>
<td></td>
<td>13.395</td>
<td>4485.1</td>
</tr>
</tbody>
</table>
**FIGURE 17.1.177.1** Logarithm of vapor pressure versus reciprocal temperature for triallate.
17.1.1.78 Triclopyr

Common Name: Triclopyr
Synonym: Garlon, Truflon, Crossbow
Chemical Name: 3,5,6-trichloro-2-pyridinylxyloxyacetic acid
CAS Registry No: 56335-06-3
Uses: herbicide
Molecular Formula: C₇H₄Cl₃NO₃
Molecular Weight: 256.471

Melting Point (°C):
148–150 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)
150.5 (Tomlin 1994)

Boiling Point (°C):
290 (dec., Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm³ at 20°C):

Dissociation Constant pKₐ:
2.68 (Spencer 1982; Worthing & Walker 1987)
2.93 (Woodburn et al. 1993)
3.97 (Tomlin 1994)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
102.5 (Rordorf 1989)

Enthalpy of Fusion, ΔH₅₇ (kJ/mol):
31.8 (Rordorf 1989)

Entropy of Fusion, ΔS₅₇ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₅₇ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
430 (Kenaga 1980a,b)
440 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)
408 (20°C, Tomlin 1994)
7690, 8100, 8220 (20°C, at pH 5, 7, and 9, Tomlin 1994)
7618 (20–25°C, quoted as 2.97E + 01 mol/m³, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.6 × 10⁻⁴ (Spencer 1982)
1.68 × 10⁻⁴ (Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)
1.90 × 10⁻³, 1.0 × 10⁻¹, 0.031, 0.59, 7.80 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pa) = 17.65 – 6672.3/(T/K); measured range 85.4–145°C (gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pa) = 14.445 – 5354.8/(T/K); measured range 150–186°C (gas saturation-GC, Rordorf 1989)
2.0 × 10⁻⁴ (vapor pressure balance, Tomlin 1994)
2.91 × 10⁻³ (20–25°C, Majewski & Capel 1995)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

Octanol/Water Partition Coefficient, log Kₐw:
−0.52 (Kenaga 1980a)
0.42, −0.45, −0.96 (pH 5, 7, and 9, Tomlin 1994)
1.30 (Isensee 1991)
2.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Herbicides

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_{p}$:
1.49, –0.22 (fish: flowing water tests, static ecosystem tests, Kenaga 1980a)
1.30, 0 (fish: calculated-solubility, $K_{OW}$, Kenaga 1980b)

Sorption Partition Coefficient, log $K_{OC}$:
1.43 (soil, Kenaga 1980a)
1.43, 2.204 (soil: quoted, calculated, Kenaga 1980b)
1.43, 2.20 (soil, Bottoni & Funari 1992)
1.43 (quoted or calculated-MCI $\chi$, Sabljic et al. 1995)

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

Volatilization:
Photolysis: photolysis $t_{1/2} < 0.4$ d in sterile, pH 5-buffered water at 40°N latitude in midday, midsummer (McCall & Gavit 1986);
photodecomposition $t_{1/2} < 12$ h (Worthing 1987; Tomlin 1994);
photodecomposition $t_{1/2} < 24$ h (Hartley & Kidd 1987);
aqueous photolysis pseudo-first order $t_{1/2}$(average) = 0.5 and 1.3 d in pH 7-buffered water and natural river water, respectively, at 25°C under artificial lights and midsummer sunlight, 40°N latitude (Woodburn et al. 1993);
aqueous photolysis rate constant, $k = 8.3 \times 10^{-2}$ h$^{-1}$ (Armbrust 2000).

Oxidation:
Hydrolysis: hydrolysis $t_{1/2} > 3$ months in darkened, sterile, buffered water at pH of 5–9 and 25°C (Woodburn et al. 1993);
stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 4.3 \times 10^{12}$ M$^{-1}$·h$^{-1}$ (Armbrust 2000).

Biodegradation: in soil, fairly rapid degradation by microbial activity, with an average $t_{1/2} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);
aerobic rate constant, $k = 9.03 \times 10^{-4}$ h$^{-1}$ (Armbrust 2000).

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

Half-Lives in the Environment:

Air:
Surface water: stable to hydrolysis, but subject to photolysis with $t_{1/2} < 12$ h (Spencer 1982; Worthing 1987; Tomlin 1994);
photolysis $t_{1/2} < 0.4$ d in sterile, pH 5 buffered water at 40°N latitude (McCall & Gavit 1986);
$t_{1/2} \sim 3$ to 4 d in natural water during summer conditions (Solomon et al. 1988);
pseudo-first order photolysis $t_{1/2}$(ave.) = 0.5 and 1.3 d in pH-buffered water and natural river water, respectively; the photodegradation pseudo-first-order half-lives in sterile, pH 7 water, midsummer sunlight at 40°N latitude and 25°C calculated as $k = 0.36$ (0.33–0.39) and 0.60 (0.50–0.70) d under artificial and natural sunlight, respectively; $t_{1/2} = 0.71$ (0.70–0.73) and 1.86 (1.77–1.96) d in river water under artificial and natural sunlight conditions, respectively, in midsummer sunlight and approximately 40°N latitude and 25°C (Woodburn et al. 1993);
photodecomposition $t_{1/2} < 24$ h (Hartley & Kidd 1987).

Ground water: reported half-lives or persistence, $t_{1/2} = 40$ and 46 d (Bottoni & Funari 1992).

Sediment:
Soil: fairly rapid degradation by microbial activity, with an average $t_{1/2} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);

Biota:
17.1.1.79 Trifluralin

Common Name: Trifluralin
Synonym: Agreflan, Crisalin, Digermin, Elancolan, L-36352, Nitran, Nitrofor, Olibref, Treflan, Trifluoramine, Trifurex, Trikepin, Trim

Chemical Name: 2,6-dinitro-N,N-dipropyl-4-trifluoromethylaniline; 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine

Uses: pre-emergence herbicide to control many grass and broadleaf weeds.

CAS Registry No: 1582-09-8
Molecular Formula: C\textsubscript{13}H\textsubscript{16}F\textsubscript{3}N\textsubscript{3}O\textsubscript{4}
Molecular Weight: 335.279

Melting Point (°C):
49 (Lide 2003)
Boiling Point (°C):
362 (estimated, Grain 1982)
139–140 (at 4.2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
96–97 (at 0.18 mmHg, Herbicide Handbook 1989)

Density (g/cm\textsuperscript{3} at 20°C):
1.294 (25°C, Montgomery 1993)
1.36 (22°C, Tomlin 1994)

Molar Volume (cm\textsuperscript{3}/mol):
295.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK\textsubscript{a};

Enthalpy of Vaporization, ∆H\textsubscript{v} (kJ/mol):
8754 (Rordorf 1989)

Enthalpy of Fusion, ∆H\textsubscript{fus} (kJ/mol):
23.85 (DSC method, Plato & Glasgow 1969)
23.5 (Rordorf 1989)

Entropy of Fusion, ∆S\textsubscript{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S\textsubscript{fus} = 56 J/mol K), F: 0.581 (mp at 49°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
24 (27°C, Woodford & Evans 1963; Günther et al. 1968; Spencer 1973)
40 (29.5°C, Melnikov 1971)
0.35 (20°C, Weber 1972; Worthing & Walker 1987)
0.1–0.5 (Probst et al. 1975)
0.60 (Herbicide Handbook 1978; Kenaga 1980; Kenaga & Goring 1980)
0.05 (Wauchope 1978; Weber et al. 1980)
< 1.0 (20°C, Khan 1980)
0.30 (Beste & Humburg 1983; Jury et al.1984; Taylor & Glotfelty 1988; Herbicide Handbook 1989)
0.32 (generator column-HPLC-RI, Swann et al. 1983)
0.70 (HPLC-RT correlation, Swann et al. 1983)
4.0 (27°C, Verschueren 1983; Montgomery 1993)
0.75 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
< 1.0 (27°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
0.30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.184, 0.221, 0.189 (at pH 5, 7, 9, Tomlin 1994)
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):

0.0265 (29.5°C, Probst et al. 1967; Khan 1980)
0.0292 (29°C, effusion method, Hamaker & Kerlinger 1971)
0.0138 (20°C, Weber 1972; Worthing & Walker 1987)
0.0323 (30°C, from Spencer & Clath 1973 unpublished data, Spencer et al. 1973)
0.0065* (20°C, gas saturation-GC, measured range 20–40°C, Spencer & Clath 1974, Spencer 1976)
\[ \log (P/\text{mmHg}) = 17.318 - 6344/(T/K) \] temp range 20–40°C (Antoine eq., Spencer 1976)
0.0262 (30°C, effusion method-pressure gauge, DePablo 1976)
0.0137 (Worthing & Walker 1979, Worthing & Hance 1991; Hartley & Kidd 1987)
0.0029 (20–25°C, Weber et al. 1980)
0.0173 (Herbicide Handbook 1983)
0.015 (20°C, Jury et al. 1983)
0.0147 (Herbicide Handbook 1989)
0.010* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
\[ \log (P/P_a) = 17.46 - 5800.6/(T/K) \] measured range 48.8–124°C (solid, gas saturation-GC, Rordorf 1989)
\[ \log (P/P_a) = 13.65 - 4573.1/(T/K) \] measured range 48.8–124°C (liquid, gas saturation-GC, Rordorf 1989)
0.015 (20°C, selected, Taylor & Spencer 1990)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0147 (20°C, Montgomery 1993)
0.0095 (Tomlin 1994)
0.0363 (liquid Pa, GC-RT correlation; Donovan 1996)

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

4.02 (20°C, calculated-P/C, Suntio et al. 1988)
16.36 (calculated-P/C, Taylor & Glotfelty 1988)
5.206 (fog chamber-GC/ECD, Fendinger et al. 1989)
5.95 (wetted-wall column-GC/ECD, Fendinger et al. 1989)
16.0 (calculated-P/C, Nash 1989)
13.27 (20°C, calculated-P/C, Muir 1991)
4.903 (23°C, calculated-P/C, Montgomery 1993)
15.2, 6.67, 4.02 (quoted literature values, Grover et al. 1997)
10.31, 15.06 (20°C, distilled water, salt water 33.3% NaCl, wetted wall column-GC, Rice et al. 1997b)
\[ \log K_{AW} = -1546/(T/K) + 2.87 \] temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
\[ \log K_{AW} = -1232/(T/K) + 1.94 \] temp range 8.3–43.5°C, (salt water solution, 33.3% NaCl, wetted-wall column-GC, Rice et al. 1997b)
11.16, 11.04; 12.50 (20°C, microlayer, subsurface natural water of salinity 17% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
10.97, 10.72; 12.38 (20°C, microlayer, subsurface natural water of salinity 16% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
10.40, 10.06; 11.82 (20°C, microlayer, subsurface natural water of salinity 12%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
12.43, 12.70; 14.84 (20°C, microlayer, subsurface water of salinity 32%, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
9.49, 13.14, 19.67 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
8.50, 12.80; 19.61 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
8.87, 12.26, 19.69 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
7.95, 12.04; 19.40 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)
6.99, 9.94, 15.85 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)  
log \( K_{AW} = -786/(T/K) + 0.307 \); temp range: 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)  
log \( K_{AW} = -1232/(T/K) + 1.900 \); temp range: 8.3–43.5°C, (subsurface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)  
4.026 (calculated-P/C, this work)  
9.63 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)  
\( \log K_{AW} = 2.870 - 1546/(T/K) \), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)  

Octanol/Water Partition Coefficient, \( \log K_{OW} \):  
5.34 (Kenaga & Goring 1980)  
3.06 (Rao & Davidson 1980)  
5.34 (shake flask-UV, Briggs 1981)  
5.28 (shake flask, Brown & Flagg 1981)  
3.97 (shake flask-GC, Kanazawa 1981)  
4.94 (HPLC-k’ correlation, McDuffie 1981)  
4.86 (shake flask, Dubelman & Bremer 1983)  
4.19 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)  
5.07, 5.28, 5.34 (Montgomery 1993)  
4.88 (RP-HPLC-RT correlation, Saito et al. 1993)  
4.82 (RP-HPLC-RT correlation, Sichaldi & Finizio 1993)  
5.34 (recommended, Sangster 1993; Hansch et al. 1995)  
5.27 (pH 7.7–8.9, Tomlin 1994)  
5.13 (Pomona-database, Müller & Kördel 1996)  
4.82 (RP-HPLC-RT correlation, Finizio et al. 1997)  
4.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)  

Bioconcentration Factor, \( \log BCF \):  
3.97, 3.66 (measured, Metcalf & Sanborn 1975)  
3.51, 3.03 (fathead minnow, kinetic test, chronic exposure, Spacie & Hamelink 1979)  
3.11 (mosquito fish, correlated-S, Spacie & Hamelink 1979)  
3.01 (rainbow trout, correlated-\( K_{OW} \), Spacie & Hamelink 1979)  
3.26–3.76 (Spacie & Hamelink 1979)  
3.66, 3.04 (quoted exppl., calculated-\( K_{OC} \), Kenaga 1980)  
2.92 (calculated-S, Kenaga 1980)  
2.95 (calculated-\( K_{OC} \), Briggs 1981)  
3.50 (Pseudorasbora parva, Kanazawa 1981)  
3.26–3.76 (selected, Schnoor & McAvoy 1981; Schnoor 1992)  
2.67, 5.02 (dry leaf, wet leaf, Bacci et al. 1990)  

Sorption Partition Coefficient, \( \log K_{OC} \):  
4.14 (soil, Harvey 1974; Kenaga 1980; Kenaga & Goring 1980)  
3.76 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
3.64 (av. 3 soils, McCull et al. 1980)  
4.49 (Georgia’s Hickory Hill pond sediment, Brown & Flagg 1981)  
2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)  
3.78 (soil, Thomas 1982)  
3.87 (soil average, Jury et al. 1983)  
3.63 (soil slurry method, Swann et al. 1983)  
3.98 (RP-HPLC-RT correlation, Swann et al. 1983)  
3.86 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
5.13 (RP-HPLC-k’ correlation, cyanopropyl column, Hodson & Williams 1988)  
3.59 (Nash 1988)
Herbicides 3673

2.94 (average of 2 soils, Kanazawa 1989)
3.64–4.15, 3.76–4.14 (soil, quoted values, Bottoni & Funari 1992)
4.71, 4.44, 4.59 (No. 1 and 2 soil, No. 3 soil and No. 4 soil; Francioso et al. 1992)
3.90 (soil, 20–25°C, selected, Wauchope et al. 1992)
4.37 (selected, Lohninger 1994)
3.94 (soil, HPLC-screening method; calculated-PC KOC fragment method, Müller & Kördel 1996)
3.93 (soil, calculated-PC KOC fragment method, Sabljic et al. 1995)
3.94; 3.99 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.86 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.53, 3.45, 3.96 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
4.42 (average values for sediments with OC ≥ 0.5%, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
3.87 (Grover et al. 1978)
3.63 (experimental, Grover et al. 1979)
4.14 (av. soils/sediments, Kenaga & Goring 1980)
3.90 (sorption isotherm-GC, Briggs 1981)
1.36, 2.08, 2.98 (log K_{p}; with first-order rate 0.52, 0.2, 8.3 × 10^{-3} h^{-1}, Karickhoff & Morris 1985)
4.14, 3.75 (selected, estimated, Magee 1991)
2.94–4.49 (Montgomery 1993)
4.37 (selected, Lohninger 1994)

Adsorption Coefficient K_{d} (L kg^{-1}):
8.1 (homoionic K^+-montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization: initial rate constant k = 2.6 × 10^{-2} h^{-1} and predicted rate constant k = 6.6 × 10^{-2} h^{-1} from soil with t_{1/2} = 10.5 h (Thomas 1982);
t_{1/2} = 18 d (Jury et al. 1983; quoted, Grover 1991);
measured rate constant k = 2–6 d^{-1} (Glottelfty et al. 1984; quoted, Glotflety 1989);
estimated rate constant k = 0.7 d^{-1} (Glotfeltety et al. 1989);
estimated t_{1/2} ~ 1.6 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: t_{1/2} < 1 h under acidic conditions in aqueous methanolic solution (Crosby & Leitis 1973)
k = 2.0 d^{-1} with t_{1/2} = 22 min for direct sunlight photolysis near surface water at 40°N in the summer (Zepp & Cline 1977; Zepp 1980; Zepp et al. 1984)
t_{1/2}(calc) = 0.94 h for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982)
k = 0.03 d^{-1} with t_{1/2} = 22 d for direct sunlight near surface (Schnoor & McAvoy 1981)
k = 0.028–0.012 min^{-1} corresponding to t_{1/2} = 25–60 min for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)
t_{1/2} = 0.5 h estimated from photolysis reaction rate by direct sunlight of midday in mid-summer at 40°N near surface water (Zepp 1991)
t_{1/2} ~ minutes to several months depending on the substrate under sunlight in all media (summary of literature data, Grover et al. 1997)

Oxidation:
Hydrolysis: t_{1/2}(calc) > 1yr buffered at pH 4, 7, 9 and incubated at 50°C (Grover et al. 1997)
Abiotic Transformations: Degradation by abiotic reductive transformations:
k = 1.79 × 10^{-3} min^{-1} at pH 6.5, 1.08 × 10^{-2} min^{-1} at pH 6.72–6.75, 1.64 × 10^{-2} min^{-1} at pH 6.84, 4.90 × 10^{-2} min^{-1} at pH 6.94, 7.09 × 10^{-2} min^{-1} at pH 6.97, 0.141 min^{-1} at pH 7.14, 0.390 min^{-1} at pH 7.46, 0.566 min^{-1} at pH 7.53, and 0.727 min^{-1} at pH 7.73 covering half-lives of 1–400 min., in reaction mixture of 0.5 mM Fe(II) and 100 mg/L goethite solutions (Klupinski & Chin 2003)
k = 1.88 M^{-1} s^{-1} in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

\[
k = 1.13 \times 10^{-3} \text{ h}^{-1} \text{ at pH 6.5, } k = 1.11 \times 10^{-2} \text{ h}^{-1} \text{ at pH 7.0, } k = 0.0251 \text{ h}^{-1} \text{ at pH 7.4, and } k = 3.40 \text{ h}^{-1} \text{ at pH 7.8 for aqueous ferrous ion system;}
\]

\[
k = 0.361 \text{ h}^{-1} \text{ at pH 6.5, } k = 0.750 \text{ h}^{-1} \text{ at pH 6.7, } k = 2.57 \text{ h}^{-1} \text{ at pH 7.0, and } k = 6.66 \text{ h}^{-1} \text{ at pH 7.3 for Fe(II)/goethite system; and}
\]

\[
k = 4.23 \times 10^{-3} \text{ h}^{-1} \text{ at pH 6.5, } k = 5.38 \times 10^{-3} \text{ h}^{-1} \text{ at pH 7.0, } k = 1.10 \times 10^{-2} \text{ h}^{-1} \text{ at pH 7.4 and } k = 2.36 \times 10^{-2} \text{ h}^{-1} \text{ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)}
\]

Biodegradation:

\[
t_{1/2} = 4–5 \text{ d for } 4 \mu g/mL \text{ to biodegrade in flooded soils at 24.5°C and } t_{1/2} = 21 \text{ d at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991)};
\]

\[
t_{1/2} > 20 \text{ d for } 0.33 \mu g/mL \text{ to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991)};
\]

\[
t_{1/2} = 20 \text{ d for } 0.5 \mu g/mL \text{ to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991)};
\]

Degradation \( t_{1/2} < 1 \text{ month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm trifluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)}
\]

\[
t_{1/2} < 1 \text{ month for } 1.0 \mu g/mL \text{ to biodegrade in flooded soils at 25°C (derived from Camper et al. 1980; Muir 1991)};
\]

\[
k = 0.008 \text{ d}^{-1} \text{ by soil incubation die-away test and } k = 0.025 \text{ d}^{-1} \text{ by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982)};
\]

\[
t_{1/2} = 132 \text{ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991)};
\]

\[
t_{1/2} = 46 \text{ wk for } 2.0 \mu g/mL \text{ to biodegrade in flooded soils at 25°C (Brewer et al. 1982; quoted, Muir 1991)};
\]

\[
t_{1/2} = 20 \text{ d for } 0.36 \mu g/mL \text{ to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991)};
\]

\[
k = -0.00504 \text{ to } -0.00730 \text{ h}^{-1} \text{ in nonsterile sediment, } k = -0.00160 \text{ to } -0.00651 \text{ h}^{-1} \text{ in sterile sediment by shake-tests at Range Point; } k = -0.00827 \text{ to } -0.01140 \text{ h}^{-1} \text{ in nonsterile water, and } k = -0.00499 \text{ to } -0.00712 \text{ h}^{-1} \text{ in sterile water by shake-tests at Range Point (Walker et al. 1988)};
\]

\[
k = -0.00621, -0.0121 \text{ h}^{-1} \text{ in nonsterile sediment, } k = -0.00476, -0.00409 \text{ h}^{-1} \text{ in sterile sediment by shake-tests at Davis Bayou and } k = -0.00439, -0.00349 \text{ h}^{-1} \text{ in nonsterile water, and } k = -0.00299, -0.00598 \text{ h}^{-1} \text{ in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).}
\]

Biotransformation:

Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:

Air: mean \( t_{1/2} = 42 \text{ min under August conditions in California range from 21–63 min (Woodrow et al. 1978)}
\]

\[
t_{1/2} = 25–60 \text{ min for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)};
\]

\[
t_{1/2} = 182–193 \text{ min under fall sunlight conditions in October (Woodrow et al. 1983)};
\]

Surface water: calculated \( t_{1/2} = 21 \text{ min from midday direct sunlight photolysis rate constant of } 2.0 \text{ h}^{-1} \text{ (Zepp 1978; Zepp & Cline 1977; quoted, Zepp et al. 1984)}\)

\[
calculated \ t_{1/2} = 0.94 \text{ h for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982)};
\]

\[
t_{1/2} < 20 \text{ d for } 2.5–5 \text{ cm water over flooded soils, } t_{1/2} = 20 \text{ h in water above sediment in estuarine sediment-water microcosm (Muir 1991)};
\]

\[
t_{1/2} < 9 \text{ h in buffered aqueous solution of pH 7 under Xenon lamp (quoted, Grover et al. 1997)};
\]

\[
t_{1/2} = 1–400 \text{ min in reaction mixture of } 0.5 \text{ mM and } 100 \text{ mg/L goethite solution for pHs from 6.5 to 7.73 (Klupinski & Chin 2003)};
\]

Ground water: reported \( t_{1/2} = 4–67, 57–126, 70, 83, \) and \( 105–132 \text{ d (Bottoni & Funari 1992)}\)

Sediment: degradation \( t_{1/2} = 9 \text{ d in estuarine sediment (18°/∞) system (Means et al. 1983)}\)

\[
t_{1/2} = 18.5 \text{ d in flooded sediment (quoted, Grover et al. 1997)};
\]

Soil: \( t_{1/2} = 4–5 \text{ d for } 4 \mu g/mL \text{ to biodegrade in flooded soils at 24.5°C and } t_{1/2} = 21 \text{ d at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);}
\]

\[
estimated persistence of 6 months in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
\]

\[
degradation \ t_{1/2} = 93 \text{ d in soil (Parr & Smith 1973; quoted, Means et al. 1983);}
\]
t½ > 20 d for 0.33 µg mL⁻¹ to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991); degradation t½ = 1 d (Kearney et al. 1976; quoted, Means et al. 1983); and t½ = 54 d in soil (Zimdahl & Gwynn 1977; quoted, Means et al. 1983);

t½ = 20 d for 0.5 µg/mL to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991);
persistence of more than 6 months (Wauchope 1978);

t½ < 21 d in flooded soil at 20–25°C (Golab et al. 1979)

biodegradation t½ < 1 month in 3 flooded soils at 25°C (Camper et al. 1980);
estimated first-order t½ ~ 86.6 d in soil from biodegradation rate constant k = 0.008 d⁻¹ by soil incubation
die-away test and t½ = 27.7 d in anaerobic systems from rate constant k = 0.025 d⁻¹ by flooded soil
incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);

Field studies: t½ = 9.5 wk - 1978 first study; t½ = 11.8 wk - 1978 second study; t½ = 12.2 wk –1979, in a
Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)
Laboratory studies: t½ = 19.6 wk at 4°C, t½ = 7.1 wk at 25°C for soil of field capacity moisture (27% w/w
for Crowley silt), t½ = 16.2 wk at 4°C, t½ = 3.9 wk at 25°C for flooded soils, Crowley silt loam; and

Field studies: t½ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996)
Estimated t½ ~ 25 to > 201 d under a variety of agronomic conditions in agriculture soils depending on
depth of incorporation, soil moisture, soil temperature, sil air, and soil organic matter content (summary
of literature data, Grover et al. 1997)

Biota: t½ = 22–31 d in river saugers, t½ = 17–57 d in river shorthead redhorse, t½ = 23 d in river golden redhorse,
t½ = 3 d in lab. fathead minnow (Spacie & Hamelink 1979);
biocatalytic t½ = 132 d (Jury et al. 1987a,b; Jury & Ghodrati 1989).
### TABLE 17.1.1.79.1
Reported vapor pressures of trifluralin at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th></th>
<th>Gas saturation method</th>
<th>Gas saturation-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>20</td>
<td>0.0065</td>
<td>25</td>
</tr>
<tr>
<td>30</td>
<td>0.0323</td>
<td>50</td>
</tr>
<tr>
<td>40</td>
<td>0.155</td>
<td>75</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td>125</td>
</tr>
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</table>

For solid

eq. 1 \( P_s/Pa \)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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<tbody>
<tr>
<td>A</td>
<td>17.46</td>
</tr>
<tr>
<td>B</td>
<td>5800.6</td>
</tr>
</tbody>
</table>

For liquid

eq. 1 \( P_l/Pa \)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>13.65</td>
</tr>
<tr>
<td>B</td>
<td>4573.1</td>
</tr>
</tbody>
</table>

### FIGURE 17.1.1.79.1
Logarithm of vapor pressure versus reciprocal temperature for trifluralin.
17.1.1.80 Vernolate

Common Name: Vernolate
Synonym: PPTC, R1607, Vanalate, Vernam, Vernnolaolate
Chemical Name: \( S\)-propyldipropylthiocarbamate; \( S\)-propyldipropylcarbamothioate
Uses: herbicide incorporated with soil for pre-planting or pre-emergence control of broadleaf and grass weeds in groundnuts, soybeans, maize, tobacco, and sweet potatoes.
CAS Registry No: 1929-77-7
Molecular Formula: \( C_{10}H_{21}NOS \)
Molecular Weight: 203.345
Melting Point (°C): liquid
Boiling Point (°C):
- 150 (at 30 mmHg, Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 149–150 (at 30 mmHg, Budavari 1989)
Density (g/cm³ at 20°C):
- 0.952 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
- 269.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant \( pK_a \):
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):
- 107 (Martin & Worthing 1977)
- 107 (21°C, Verschueren 1983)
- 107 (Budavari 1989; Milne 1995)
- 95 (Wauchop 1989)
Vapor Pressure (Pa at 25°C or as indicated):
- 0.84 (20°C, Hartley & Graham-Bryce 1980)
- 1.386 (Khan 1980; Spencer 1982; Herbicide Handbook 1989)
- 1.333 (Ashton & Crafts 1981)
- 0.244 (20°C, GC-RT correlation, Kim 1985)
- 1.39 (Hartley & Kidd 1987)
- 0.9 (20°C, selected, Suntio et al. 1988)
- 1.386 (Budavari 1989)
- 1.39 (Worthing & Hance 1991; Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
- 2.05 (20°C, calculated-P/C, Suntio et al. 1988)
- 2.034 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log \( K_{ow} \):
- 3.84 (20°C, Worthing & Hance 1991; Tomlin 1994)
Bioconcentration Factor, log BCF:
1.64 (calculated-S, Kenaga 1980)
1.70 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.52 (calculated-S, Kenaga 1980)
2.03, 1.93 (quoted exptl.; calculated-MCI and fragment contribution method, Meylan & Howard 1992)
2.41 (estimated-chemical structure, Lohninger 1994)
2.33 (soil, calculated-MCI $^1$,$^2$; Sabljic et al. 1995)
2.33; 2.40, 2.11 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Biodegradation: microbial degradation $t_{1/2} = 8–16$ d at 27°C, $t_{1/2} > 64$ d at 4°C in soil (Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{1/2} ~ 1.5$ wk in moist loam soil at 21–27°C (Herbicide Handbook 1989);
selected field $t_{1/2} = 12$ d (Wauchope et al. 1992; Hornsby et al. 1996);
soil $t_{1/2} = 11$ d (Pait et al. 1992);
microbial degradation $t_{1/2} = 8–16$ d at 27°C, $t_{1/2} > 64$ d at 4°C (Tomlin 1994).

Biota:
### 17.2 SUMMARY TABLES

#### TABLE 17.2.1
Common names, chemicals names and physical properties of herbicides

<table>
<thead>
<tr>
<th>Compound</th>
<th>Synonym</th>
<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW (g/mol)</th>
<th>m.p. (°C)</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>pKₐ</th>
<th>pKₐ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alachlor [15972-60-8]</td>
<td>Lasso, Metachlor</td>
<td>α-chloro-2,6-diethyl-N-methoxy-methylacetanilide</td>
<td>C₁₄H₂₀ClNO₂</td>
<td>269.768</td>
<td>40</td>
<td>0.713</td>
<td>0.62</td>
<td></td>
</tr>
<tr>
<td>Ametryn [834-12-8]</td>
<td>Evik, Gesapax</td>
<td>2-methylthio-4-(ethylamino)-6-(isopropylamino)-s-triazine</td>
<td>C₉H₁₇N₅S</td>
<td>227.330</td>
<td>88</td>
<td>0.241</td>
<td>4.00</td>
<td>10.07</td>
</tr>
<tr>
<td>Amitrole [61-82-5]</td>
<td>Amerol, Aminotriazole</td>
<td>3-amino-1H-1,2,4-triazole</td>
<td>C₇H₈N₄</td>
<td>84.080</td>
<td>159</td>
<td>0.0484</td>
<td></td>
<td>9.83</td>
</tr>
<tr>
<td>Atrazine</td>
<td>Gesaprim</td>
<td>2-chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine</td>
<td>C₁₄H₂₀ClNO₂</td>
<td>269.768</td>
<td>40</td>
<td>0.713</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Barban [101-27-9]</td>
<td>Carbyne</td>
<td>4-chlorobut-2-ynyl-3-chlorocarbanilate</td>
<td>C₁₃H₁₆NO₂</td>
<td>288.316</td>
<td>66</td>
<td>0.396</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benfluralin [1861-40-1]</td>
<td>Balan, Bonalan</td>
<td>N-butyl-N-ethyl-α,α,α-trifluoro-2,6-di-nitro-p-toluidine</td>
<td>C₁₆H₁₈N₃O₂F₃</td>
<td>335.279</td>
<td>66</td>
<td>0.396</td>
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<td></td>
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<tr>
<td>Bifenox [42576-02-3]</td>
<td>Modown</td>
<td>methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate</td>
<td>C₁₅H₁₅ClNO₅</td>
<td>342.131</td>
<td>85</td>
<td>0.258</td>
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<tr>
<td>Bromacil [314-40-9]</td>
<td>Borea, Hyvar X</td>
<td>5-bromo-3-sec-butyl-6-methyl-uracil</td>
<td>C₉H₁₉BrN₂O₂</td>
<td>261.115</td>
<td>158</td>
<td>0.0496</td>
<td>9.10</td>
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<tr>
<td>Bromacil lithium salt</td>
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<td></td>
<td>C₁₅H₁₉Br₂N₂O₂</td>
<td>261.115</td>
<td>158</td>
<td>0.0496</td>
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<td>Bromacil butyrate ester [3861-41-4]</td>
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<td>3,5-dibromo-4-hydroxybenzonitrile</td>
<td>C₁₅H₁₅BrNO</td>
<td>276.913</td>
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<td>0.0241</td>
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<tr>
<td>Bromacil octanoate ester [1689-99-2]</td>
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<td>2,6-dibromo-4-cyanophenyl octanoate</td>
<td>C₁₅H₁₉Br₂N₂O₂</td>
<td>403.109</td>
<td>45–46</td>
<td>0.629</td>
<td>4.08</td>
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<tr>
<td>Benoxynil [1689-84-5]</td>
<td>Brominal, Buctril</td>
<td>3,5-dibromo-4-hydroxybenzonitrile</td>
<td>C₁₅H₁₉Br₂N₂O₂</td>
<td>403.109</td>
<td>45–46</td>
<td>0.629</td>
<td>4.08</td>
<td></td>
</tr>
<tr>
<td>BENZ leth® [26259-45-0]</td>
<td>Etazine, Sumitol</td>
<td>N-ethyl-6-methoxy-N'-(1-methylpropyl)-1,3,5-triazine-2,4-diamine</td>
<td>C₁₅H₁₉N₂O</td>
<td>225.291</td>
<td>87</td>
<td>0.246</td>
<td>4.40</td>
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<tr>
<td>Butralin [33629-47-9]</td>
<td>Amex, Tamex</td>
<td>N-sec-butyl-4-tetra-butyl-2',6'-dinitroaniline</td>
<td>C₁₅H₂₃N₂O₄</td>
<td>295.335</td>
<td>60</td>
<td>0.454</td>
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<tr>
<td>Butylate [2008-41-5]</td>
<td>Sutan</td>
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<td>(R)-2-(2,4-dichlorophenoxy)propionic acid</td>
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<td>4-nitrophenyl α,α,α-trifluoro-2-nitrophenoxy-4-(1H)-pyridinone</td>
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<td>3-(3-chloro-4-methoxyphenyl)-1,1-dimethyleurea</td>
<td>C_{10}H_{13}ClN_{2}O_2</td>
<td>228.675</td>
<td>126-127</td>
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<tr>
<td>Metribuzin</td>
<td>Metribazine, Lexone, Preview, Sencor</td>
<td>4-amino-6-(r-butyl)-3-(methylthio)-1,2,4-triazin-5-(4H)-one</td>
<td>C_{7}H_{14}N_{2}O_{5}S</td>
<td>214.288</td>
<td>126</td>
<td>0.102</td>
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<td>Molinate [2212-67-1]</td>
<td>Ordram</td>
<td>S-ethyl azepane-1-carbothioate</td>
<td>C_{6}H_{10}N_{2}S</td>
<td>187.302</td>
<td>liquid</td>
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<td>Monolinuron [1746-81-2]</td>
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<td>3-(4-chlorophenyl)-1-methoxy-1-methylurea</td>
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<td>214.648</td>
<td>77</td>
<td>0.309</td>
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<td>Monuron [150-68-5]</td>
<td>Telvar, Urox</td>
<td>1,1-dimethyl-3-(p-chloro-phenyl)-urea</td>
<td>C_{9}H_{16}ClN_{2}O</td>
<td>198.648</td>
<td>170.5</td>
<td>0.0374</td>
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<td>Napropamide [15299–99–7]</td>
<td>Devrinol</td>
<td>2-(α-naphthloxy)-N,N-diethylpropionamide</td>
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<td>75</td>
<td>0.323 2.93</td>
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<td>Neburon [555-37-3]</td>
<td>Kloben</td>
<td>1-butyl-3-(3,4-dichlorophenyl)-1-methyl urea</td>
<td>C_{12}H_{16}Cl_{2}N_{2}O</td>
<td>275.174</td>
<td>102-103</td>
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<td>Nitrinil [4726-14-1]</td>
<td>Planavin</td>
<td>4-(methylsulfonyl)-2,6-dinitro-N,N-dipropylaniline</td>
<td>C_{5}H_{10}N_{2}O_{5}S</td>
<td>345.371</td>
<td>150</td>
<td>0.0594</td>
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<td>Nitrofen [1836–75–5]</td>
<td>nitrophen, Tok, Tokkron</td>
<td>2,4-dichloro-1-(4-nitrophenoxy)benzene</td>
<td>C_{9}H_{7}Cl_{2}N_{2}O_{3}</td>
<td>284.095</td>
<td>70</td>
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<td>Norflurazon [27314–13–2]</td>
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<td></td>
<td>C_{3}H_{7}ClF_{2}N_{O}</td>
<td>303.666</td>
<td>184</td>
<td>0.0275</td>
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<td>Oryzalin [19044-88-3]</td>
<td>Rycelan, Rycelon, Surflan</td>
<td>4-(dipropamido)-3,5-dinitrobenzenesulfonamide</td>
<td>C_{12}H_{18}N_{4}O_{6}S</td>
<td>346.359</td>
<td>141</td>
<td>0.0728 9.40 8.60</td>
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<td>Paraquat [4685-14-7]</td>
<td>Cyclone, Gramoxone</td>
<td>1,1'-dimethyl-4,4'-pyridinium</td>
<td>C_{12}H_{14}N_{2}</td>
<td>186.252</td>
<td>dec.</td>
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<td>Paraquat dichloride salt [1910–42–5]</td>
<td></td>
<td></td>
<td>C_{12}H_{14}Cl_{2}N_{2}</td>
<td>257.2</td>
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<td>&lt; 4</td>
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<td>Pebulate [1114-71-2]</td>
<td>Tillam penoxalin</td>
<td>s-propyl butylethylcarbamothioate</td>
<td>C_{10}H_{25}N_{2}O_{4}</td>
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<td>Pendimethalin [40487–42–1]</td>
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<td>N-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine</td>
<td>C_{13}H_{19}N_{2}O_{4}</td>
<td>281.308</td>
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<td>Pentachlorophenol [87–86–5]</td>
<td>PCP</td>
<td>pentachlorophenol</td>
<td>C_{6}Cl_{5}OH</td>
<td>266.336</td>
<td>174</td>
<td>0.0350 4.74</td>
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<td>Pentachlorophenol sodium salt (Pentacon)</td>
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<td>Pentamochlor [2307-68-8]</td>
<td>Solan</td>
<td>3'-choloro-2-methylvaler-p-toluidide</td>
<td>C_{7}H_{14}ClNO</td>
<td>239.741</td>
<td>85-86</td>
<td>0.255</td>
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<td>Picloram [1918-02-1]</td>
<td>Tordon</td>
<td>4-amino-3,5,6-trichloro-picolinic acid</td>
<td>C_{7}H_{12}Cl_{2}N_{2}O_{2}</td>
<td>241.459</td>
<td>218.5</td>
<td>0.126 1.90 3.60</td>
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(Continued)
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<th>Compound</th>
<th>Synonym</th>
<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>pK_a</th>
<th>pK_b</th>
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<td>Picloram-potassium</td>
<td></td>
<td>C_6H_2Cl_3KN_2O_2</td>
<td>279.6</td>
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<td>Profluralin</td>
<td>Pregard</td>
<td>N-(cyclopropylmethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzamine</td>
<td>C_14H_16F_3N_2O_4</td>
<td>347.290</td>
<td>34</td>
<td>0.816</td>
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<td>Prometon</td>
<td>Primatol,</td>
<td>2,4-bis(isopropylamino)-6-methoxy-s-triazine</td>
<td>C_8H_18N_3O</td>
<td>225.291</td>
<td>91.5</td>
<td>0.223</td>
<td>4.28</td>
<td>9.73</td>
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<td>Prometryn</td>
<td>Caparol,</td>
<td>N,N-1,3,5-triazine-2,4-diamine-bis(isopropylamino)-6-(methylthio)</td>
<td>C_8H_18N_3S</td>
<td>241.357</td>
<td>119</td>
<td>0.120</td>
<td>4.05</td>
<td>9.95</td>
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<td>Pronamide</td>
<td>Kerb,</td>
<td>3,5-dichloro-N-(1,1-dimethyl-propynyl)-benzamide</td>
<td>C_13H_10ClN_2O_2</td>
<td>216.688</td>
<td>77</td>
<td>0.309</td>
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<td>Propanil</td>
<td>Propanex,</td>
<td>N-(3,4-dichlorophenyl)-propionamide</td>
<td>C_8H_10ClN_2O_2</td>
<td>218.079</td>
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<td>Propazine</td>
<td>Gesamil,</td>
<td>2-chloro-4,6-bis(isopropylamino)-s-triazine</td>
<td>C_13H_10ClN_2O_2</td>
<td>229.710</td>
<td>213</td>
<td>0.0143</td>
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<td>12.15</td>
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<td>Propamid</td>
<td>IPC</td>
<td>isopropyl carbanilate</td>
<td>C_11H_15NO_2</td>
<td>179.216</td>
<td>90</td>
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<td>Pyrazon</td>
<td>Chloridazon</td>
<td>5-amino-4-chloro-2-phenyl-3(2H)-pyridazine</td>
<td>C_11H_15NO_2</td>
<td>221.643</td>
<td>205</td>
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<td>Simazine</td>
<td>Gesatop,</td>
<td>2-chloro-4,6-(diethylamino)-s-triazine</td>
<td>C_13H_10ClN_2O_2</td>
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<td>12.35</td>
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<td>Simetryne</td>
<td>Gy-bon</td>
<td>N,N'-diethyl-6-methylthio-1,3,5-triazine-2,4-diyldiamine</td>
<td>C_13H_10ClN_2O_2</td>
<td>171.283</td>
<td>82-83</td>
<td>0.273</td>
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<td>2,4,5-T</td>
<td>Gesatop</td>
<td>2,4,5-trichlorophenoxyacetic acid</td>
<td>C_13H_10ClO_3</td>
<td>255.483</td>
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<td>2,3,6-TBA</td>
<td>Tysbren,</td>
<td>2,3,6-trichlorobenzoic acid</td>
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<td>225.457</td>
<td>124.5</td>
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<td>Terbacil</td>
<td>Sinbar</td>
<td>3-tert-butyl-5-chloro-6-methyluracil</td>
<td>C_13H_10ClN_2O_2</td>
<td>216.664</td>
<td>176</td>
<td>0.0330</td>
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<td>Terbumeton</td>
<td>Caragard</td>
<td>N-tert-butyl-N'-ethyl-6-methoxy-1,3,5-triazine</td>
<td>C_13H_10ClN_2O_2</td>
<td>225.290</td>
<td>123-124</td>
<td>0.108</td>
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<td>Terbutylazine</td>
<td>Gardoprim</td>
<td>N-tert-butyl-6-chloro-N'-ethyl-1,3,5-triazine-2,4-diamine</td>
<td>C_13H_10ClN_2O_2</td>
<td>229.710</td>
<td>178</td>
<td>0.0320</td>
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<td>Terbutryn</td>
<td>Igran,</td>
<td>N-tert-butyl-N'-ethyl-6-methyl-thio-1,3,5-triazine-2,4-diamine</td>
<td>C_13H_10ClN_2O_2</td>
<td>241.357</td>
<td>104</td>
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<td>Clarosan</td>
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<td></td>
<td>Prebane</td>
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<td>Herbicides</td>
<td>Commercial Names</td>
<td>Chemical Structure</td>
<td>Molecular Formula</td>
<td>Molecular Weight</td>
<td>Solubility</td>
<td>pKa</td>
<td>pKb</td>
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<td>Thiobencarb</td>
<td>Benthiocarb, Bolero, Saturno</td>
<td>S-4-chlorobenzyl-diethyl-thiocarbamate</td>
<td>C_{13}H_{10}ClNOS</td>
<td>257.779</td>
<td>1.7</td>
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<td>Triallate [2303-17-5]</td>
<td>Avadex BW, Far-Go</td>
<td>S-(2,3,3-trichloro-2-propenyl)-bis(1-methylene)carbamothioate</td>
<td>C_{10}H_{16}Cl_{2}NOS</td>
<td>304.664</td>
<td>29</td>
<td>0.914</td>
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<td>Triclopyr [55335–06–3]</td>
<td>Garlon, Trufon, Crossbow</td>
<td>3,5,6-trichloro-2-pyridinloyxyacetic acid</td>
<td>C_{7}H_{4}Cl_{3}NO_{3}</td>
<td>256.471</td>
<td>148–150</td>
<td>0.0607</td>
<td>2.68</td>
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<td>Trifluralin [1582-09-8]</td>
<td>Treflan, Triflurex, Elancolan</td>
<td>2,6-dinitro-N,N-dipropyl-4-trifluoromethylaniline</td>
<td>C_{13}H_{16}F_{3}N_{3}O_{3}</td>
<td>335.279</td>
<td>49</td>
<td>0.581</td>
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<td>Vernolate [1929-77-7]</td>
<td>Surpass, Vernam</td>
<td>S-propyldipropyliothiocarbamate</td>
<td>C_{10}H_{21}NOS</td>
<td>203.345</td>
<td>liquid</td>
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Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator
pK_{a} – acid dissociation constant; pK_{b} – basicity constant
(a) ester is quickly converted to parent acid.
* Assuming ΔS_{fu} = 56 J/mol K.
TABLE 17.2.2
Summary of selected physical-chemical properties of herbicides at 25°C

<table>
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<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Solubility</th>
<th>Henry's law constant</th>
<th>log KOC reported</th>
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<td></td>
<td>P/μPa</td>
<td>S/(g/m³)</td>
<td>C/(mol/m³)</td>
<td>C/(mol/m³)</td>
<td>H/(Pa·m³/mol)</td>
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<tr>
<td></td>
<td>P/μPa</td>
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<tr>
<td>Alachlor</td>
<td>0.0020</td>
<td>240</td>
<td>0.890</td>
<td>1.281</td>
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<td>Ametryn</td>
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<td>185</td>
<td>0.814</td>
<td>3.191</td>
<td>2.58</td>
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<td>Atrazine</td>
<td>5.50 × 10⁻⁷*</td>
<td>280000</td>
<td>3330</td>
<td>68850</td>
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<td>Barban</td>
<td>5.00 × 10⁻⁵</td>
<td>30</td>
<td>0.139</td>
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<td>Benefin</td>
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<td>11</td>
<td>0.043</td>
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<td>Bifenox</td>
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<td>0.0010</td>
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<td>Bromacil</td>
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<td>815</td>
<td>3.121</td>
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<td>Bromacil lithium salt</td>
<td>4.13 × 10⁻⁵</td>
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<td>Bromoxynil</td>
<td>6.40 × 10⁻⁴</td>
<td>130</td>
<td>0.469</td>
<td>22.54</td>
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<td>Bromoxynil octanoate</td>
<td>6.40 × 10⁻⁴</td>
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<td>sec-Bumeton</td>
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<td>11.31</td>
<td>3.52 × 10⁻⁴ 2.30</td>
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<td>Butachlor</td>
<td>6.00 × 10⁻⁴</td>
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<td>Butralin</td>
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<td>0.0034</td>
<td>7.69 × 10⁻³</td>
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<td>Chlorbromuron</td>
<td>5.33 × 10⁻⁵</td>
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<td>0.170</td>
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<td>3.13 × 10⁻⁴ 2.7</td>
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<td>Chlorfenac</td>
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<td>Chlorpropham</td>
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<td>0.417</td>
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<td>Chlorosulfuron</td>
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<td>19.56</td>
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<td>Chlortoluron</td>
<td>1.70 × 10⁻⁵</td>
<td>70</td>
<td>0.329</td>
<td>5.418</td>
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<td>Cyanazine</td>
<td>2.13 × 10⁻⁷</td>
<td>171</td>
<td>0.710</td>
<td>18.03</td>
<td>2.22</td>
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<td>2,4-D</td>
<td>8.00 × 10⁻⁵*</td>
<td>400</td>
<td>1.810</td>
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<td>4.026</td>
<td>55.92</td>
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<td>0.0019</td>
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<td>MCPA ester</td>
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<td>620</td>
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<th>Henry's law constant</th>
<th>Selected properties</th>
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<th>Selected properties</th>
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<td>P/C</td>
<td>log K_{OC}</td>
<td>reported</td>
<td>H/(Pa·m²/mol)</td>
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<td>2.33 × 10⁻³</td>
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<td>9.90 × 10⁻⁴</td>
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<td>2.18</td>
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<td>3.55 × 10⁻⁴</td>
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<td>4.49 × 10⁻⁵</td>
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<td>1.53 × 10⁻⁵</td>
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<td>90</td>
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Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator, H - herbicide

2,4-D(a) physical-chemical properties modified from values used in Vol. IV.

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to large error.
### TABLE 17.2.3
Suggested half-life classes of herbicides in various environmental compartments 25°C

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<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
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<td>5</td>
<td>6</td>
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<td>6</td>
<td>6</td>
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<tr>
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<td>4</td>
<td>4</td>
<td>5</td>
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<td>6</td>
<td>7</td>
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<th>Range (hours)</th>
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<td>2</td>
<td>17 (~ 1 day)</td>
<td>10–30</td>
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<td>3</td>
<td>55 (~ 2 days)</td>
<td>30–100</td>
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<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
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<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>
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Smith, A.E. (1979) Soil persistence experiments with (14C) 2,4-D in herbicidal mixtures and field persistence studies with triallate and trifluralin both singly and combined. *Weed Res.* 19, 165–170.


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18 Insecticides

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18.1.1 INSECTICIDES

18.1.1.1 Acephate

Common Name: Acephate
Synonym: Chevron RE 12420, ENT 27822, Orthene, Ortho 12420, Ortran, Ortril, RE 12420, 75 SP, Tornado
Chemical Name: acetylphosphorimidothioic acid O,S-dimethyl ester; O,S-dimethyl acetylphosphorimidothioate;
N-[methoxy(methylthio)phosphinoyl]acetamide
Uses: systemic insecticide with contact and stomach action to control a wide range of chewing and sucking insects in
fruit, cotton, hops, vines, soybeans, olives, groundnuts, beet, brassicas, celery, potatoes, rice ornamentals, forestry
and other crops; also used as a cholinesterase inhibitor.

CAS Registry No: 30560-19-1
Molecular Formula: C₅H₁₀NO₃PS
Molecular Weight: 183.166
Melting Point (°C): 88
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ:
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: 0.241 (mp at 88°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
> 5000 (20°C, shake flask-GC, Bowman & Sans 1983a)
790000 (20°C, Hartley & Kidd 1987)
818000 (Wauchope 1989)
790000 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
2.26 × 10⁻⁴ (20°C, Hartley & Kidd 1987)
2.27 × 10⁻⁴ (20°C, Montgomery 1993)
0.513; 0.759, 0.457 (gradient GC method; estimation using modified Watson method: Sugden’s parachor,
McGowan’s parachor, Tsuzuki 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
5.27 × 10⁻⁸ (20–25°C, calculated-P/C, Montgomery 1993)
5.06 × 10⁻⁸ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log Kᵪᵢₕ:
−0.85 (shake flask, Log P Database, Hansch & Leo 1987)
−1.87 (calculated, Montgomery 1993)
Bioconcentration Factor, log BCF:
-0.523 (calculated-S, Kenaga 1980)
0.053 (wet wt. basis, rainbow trout, Geen et al. 1984)

Sorption Partition Coefficient, log K_{OC}:
0.477 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
0.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996)
0.48 (Montgomery 1993)
0.30 (estimated-chemical structure, Lohninger 1994)
3.50, 3.00 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants or Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: calculated rate constant k \approx 51 \times 10^{-12} \text{ cm}^3/\text{molecules for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).}
Hydrolysis: persistent to hydrolysis between pH 4.0 and 6.0 under laboratory condition at 20 and 30°C regardless of temperature while strongly affected by temperature at pH 8.2; and more persistent in pond than creek water (Szeto et al. 1979)
t_{1/2} = 60 \text{ h at pH 9 and } t_{1/2} = 710 \text{ h at pH 3 both at 40°C (Montgomery 1993)}.
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: resistant to hydrolysis in distilled, buffered water at pH 4.0 to 6.9, but not at pH 8.2; and more persistent in pond than creek water, 45% found after 50 d when incubated at 9°C in creek water (Szeto et al. 1979)
Ground water:
Sediment: degradation increased greatly when treated samples were incubated in the presence of sediments, ~ 20% recovered after 42 d and ~ 28% recovered after 58 d after incubating acephate-treated pond and creek water with their respective sediments (Szeto et al. 1979)
Soil: selected field t_{1/2} = 3.0 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);
t_{1/2} = 7–10 d in soil (Tomlin 1994).
Biota:
Insecticides

18.1.1.2 Aldicarb

Common Name: Aldicarb
Synonym: Ambush, Carbanolate, ENT 27093, NCI-C08640, matadan, OMS 771, Pounce, Temik, Union Carbide 21149
Chemical Name: 2-methyl-2-(methylthio)propionaldehyde O-(methylcarbamoyl) oxime; 2-methyl-2-(methylthio)propionaldehyde O-(methylamino)carbonyl oxime
Uses: systemic insecticide, acaricide, and nematocide with contact and stomach action; also used as cholinesterase inhibitor.
CAS Registry No: 116-06-3
Molecular Formula: C₇H₁₄N₂O₂S
Molecular Weight: 190.263
Melting Point (°C):
99 (Lide 2003)
Boiling Point (°C):
100 (decomposes above this temp., Howard 1991)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
224.3 (calculated-Compiled method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ∆Hᵥₐ (kJ/mol):
25.94 (DSC method, Plato & Glasgow 1969)
Entropy of Fusion, ∆Sᵥₐ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sᵥₐ = 56 J/mol K), F: 0.188 (mp at 99°C)
Water Solubility (g/m³ or mg/L at 25°C):
4000 (24°C, shake flask-GC, Felsot & Dahm 1979)
7800 (Kenaga 1980a; Kenaga & Goring 1980)
6000 (Khan 1980; Verschueren 1983)
6016, 6000 (exptl., corrected-mp, Briggs 1981)
6000 (20°C, shake flask-GC, Bowman & Sans 1983b)
5730 (Seiber 1987)
4930 (20°C at pH 7, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
6.67 (20°C, Khan 1980)
0.00707 (20°C, selected exptl. value, Kim 1985)
0.102, 0.016 (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
0.013 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.013 (selected, Suntio et al. 1988)
0.013 (Worthing & Hance 1991)
0.004 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0046 (Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C):
2.48 × 10⁻⁴ (Jury et al. 1987a, Jury & Ghodrati 1989)
3.20 × 10⁻⁴ (calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log $K_{ow}$:

- 0.85 (shake flask, Felsot & Dahm 1979)
- 1.10 (Hansch & Leo 1979)
- 1.57 (shake flask-UV, Lord et al. 1980)
- 0.70 (Rao & Davidson 1980)
- 1.57 (20°C, shake flask-UV, Briggs 1981)
- 1.13 (20°C, shake flask-GC, Bowman & Sans 1983b)
- 1.13 (Hansch & Leo 1985)
- 0.70, 1.13 (Montgomery 1993)
- 1.13 (recommended, Sangster 1993)
- 1.13 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log $BCF$:

- 1.62 (fish in static water, Metcalf & Sanborn 1975; Kenaga & Goring 1980)
- 0.85 (vegetation, correlated-$K_{ow}$, Iwata et al. 1977; Maitlen & Powell 1982)
- 0.602 (calculated-S, Kenaga 1980; quoted, Howard 1991)
- 1.64 (earthworm, Lord et al. 1980; quoted, Connell & Markwell 1990)
- 1.00, 1.18 (log $BCF_{lipid}$, log $BCF_{protein}$, Briggs 1981)

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

- 1.36–1.57 (Felsot & Dahm 1979)
- 0.91, 1.20 (Bromilow & Leistra 1980)
- 1.51 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 1.39 (reported as log $K_{OM}$, Briggs 1981)
- 1.51 (estimated, Kenaga 1980; quoted, Howard 1991)
- 1.30–1.40 (Bilkert & Rao 1985; quoted, Howard 1991)
- 1.56 (soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 0.85–1.67 (Montgomery 1993)
- 1.48 (estimated-chemical structure, Lohninger 1994)
- 1.50 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.40, 1.97 (estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 1.30 (soil: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

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

Volatile:

Oxidation:

- rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO\textsubscript{3}}$ with NO\textsubscript{3} radical and $k_{O_3}$ with O\textsubscript{3} or as indicated, *data at other temperatures see reference:

- photooxidation $t_{1/2} = 1$–9.5 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

- $t_{1/2} = 1.7$–12 d in soil for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard et al. 1991)

- $k(aq.) = 5.9 \times 10^6$ M\textsuperscript{-1} s\textsuperscript{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

- $k(aq.) = (4.4 \pm 0.1) \times 10^4$ M\textsuperscript{-1} s\textsuperscript{-1} for direct reaction with ozone in water at pH 2.1; $k = (4.3 \pm 0.2) \times 10^3$ M\textsuperscript{-1} s\textsuperscript{-1} at pH 7.0 and 24 ± 1°C, with $t_{1/2} = 0.08$ s at pH 7 (Yao & Haag 1991).

- $k(aq.) = (8.1 \pm 1.1) \times 10^6$ M\textsuperscript{-1} s\textsuperscript{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at 24 ± 1°C (Haag & Yao 1992)
Hydrolysis: 
- $t_{1/2} = 23$ d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991)
- $t_{1/2} = 9.9$ d at pH 6.3–7.0 at 15°C (Bromilow & Leistra 1980; quoted, Howard 1991)
- $t_{1/2} = 4580$ d, based on a first-order $k = 1.51 \times 10^{-4}$ d$^{-1}$ at pH 5.5 and 5°C (Hansen & Spiegel 1983; quoted, Howard et al. 1991)
- $t_{1/2} = 4.0$ min at pH 12.9, $t_{1/2} = 1.3$ min at pH 13.39 and 15°C (Lemley & Zhong 1983)
- $t_{1/2} = 0.4–3.2$ d in soil at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991)
- Pseudo-first order $k = 5.3 \times 10^{-3}$ d$^{-1}$ with $t_{1/2} = 131$ d at pH 3.95, $k = 1.3 \times 10^{-3}$ d$^{-1}$ with $t_{1/2} = 559$ d at pH 6.02, $k = 2.1 \times 10^{-3}$ d$^{-1}$ with $t_{1/2} = 324$ d at pH 7.96, $k = 1.3 \times 10^{-2}$ d$^{-1}$ with $t_{1/2} = 55$ d at pH 8.85 in period of 89 d; and $k = 1.2 \times 10^{-1}$ d$^{-1}$ with $t_{1/2} = 6$ d at pH 9.85 for period of 15 days at 20°C in pH-buffered distilled water (Given & Dierberg 1985; Mink et al. 1989)
- For pH buffered distilled water at 20°C: $t_{1/2} = 131$ d at pH 3.95, $t_{1/2} = 559$ d at pH 6.02, $t_{1/2} = 324$ d at pH 7.96, $t_{1/2} = 55$ d at pH 8.85, and $t_{1/2} = 6$ d at pH 9.85 (Montgomery 1993)
- $t_{1/2} = 16$ d in aqueous montmorillonite suspensions (10 g/L) at pH 3.7 (Wei et al. 2001).

Biodegradation:
- $k = 0.000222$ h$^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233$ h$^{-1}$ for discharge rate of 61 cm/year with $t_{1/2} = 30$ d (Jones & Back 1984)

Aerobic mineralization:
- $k = (1.93–34.2) \times 10^{-3}$ d$^{-1}$ with $t_{1/2} = 20–361$ d in surface soils and $k = 2.97–5.28) \times 10^{-3}$ d$^{-1}$ with $t_{1/2} = 131–233$ d in subsurface soils; anaerobic mineralization $k = (8.09–31.1) \times 10^{-4}$ d$^{-1}$ with $t_{1/2} = 223–1130$ d in surface soils after 63 d incubation (Ou et al. 1985)
- $t_{1/2} = 70$ d in 0–10 cm depth of soil (Jury et al. 1987a, b; Jury & Ghodrati 1989).

Ground water: $t_{1/2} = 960–15240$ h, based on estimated aqueous aerobic biodegradation half-life and water grab sample data (Miles & Delfino 1985; quoted, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 1–9.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991; Howard et al. 1991).

Surface water: $t_{1/2} = 5$ d in pond water, $t_{1/2} = 6$ d in lake water (Moorefield 1974; Mink et al. 1989)

Hydrolysis $t_{1/2} = 6$ to 131 d in pH-buffered distilled water at 20°C (Given & Dierberg 1985)

Aerobic biodegradation: $t_{1/2} = 480–8664$ h, based on unacclimated aerobic soil grab sample data; $t_{1/2} = 480–8664$ h, based on anaerobic ground water grab sample data (Howard et al. 1991)

Ground water: $t_{1/2} = 960–15240$ h, based on estimated aerobic biodegradation half-life and water grab sample data (Miles & Delfino 1985; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 9, 7, 12$ d in clay, silty clay loam and fine sandy loam at an application rate of 20 ppm (Coppedge et al. 1967; quoted, Montgomery 1993); hydrolysis $t_{1/2} = 23$ d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991), $t_{1/2} = 9.9$ d at pH 6.3–7.0 at 15°C (Bromilow et al. 1980; Bromilow & Leistra 1980; quoted, Howard 1991; Montgomery 1993); $t_{1/2} = 0.4–3.2$ d at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991); degradation rate constants $k = 0.000222$ h$^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233$ h$^{-1}$ for discharge rate of 61 cm/year with $t_{1/2} = 30$ d (Jones & Back 1984); mineralization $t_{1/2} = 20–361$ d in surface soils and $t_{1/2} = 131–233$ d in surface soils under aerobic condition, anaerobic $t_{1/2} = 223–1130$ d in surface soils after 63 d incubation (Ou et al. 1985) reported $t_{1/2} = 70$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993); oxidation $t_{1/2} = 1.7–12$ d for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991); rapidly oxidized to sulfoxide with $t_{1/2} = 7$ d in some soils, much more slowly to sulfone, pH dependent with $t_{1/2}$ varying from a few minutes at a pH of > 12 to ~ 560 d at a pH of 6.0. $t_{1/2}$ from 2 to > 8 wk in laboratory experiment, and $t_{1/2} < 1$ wk in field studies (Mink et al. 1989) $t_{1/2} \leq 2$ wk, field study over 218–d period in the unsaturated zone beneath a citrus grove (Hornsby et al. 1990).
$t_{1/2} = 480–8664$ h, based on unacclimated aerobic soil grab sample data (Howard 1991); selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996); $t_{1/2}$ between 0.3 and 3.5 months in surface soils (Jones & Norris 1998); $t_{1/2} = 12.0$ d in sterile soil, $t_{1/2} = 2.7$ d in non-sterile soil; $t_{1/2} = 1.6$, 1.4 and 1.7 d in soil grown with corn, mung bean and cowpea, respectively (Sun et al. 2004)

Biota: biochemical $t_{1/2} = 70$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).
18.1.1.3 Aldrin

Common Name: Aldrin
Synonym: Aldrec, Aldrex, Aldrime, Aldrosol, Altox, Compound 118, Drinox, ENT 15949, HHDN, NA 2761, NA 2762, Octalene, Seedrin
Chemical Name: 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endoexo-5,8-dimethano-naphthalene
Uses: Insecticide/Fumigant
CAS Registry No: 309-00-2
Molecular Formula: C₁₂H₈Cl₆
Molecular Weight: 364.910
Melting Point (°C):
  104  (Lide 2003)
Boiling Point (°C):
  145  (at 2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
Density (g/cm³ at 20°C):
  1.70  (Montgomery 1993)
Molar Volume (cm³/mol):
  316.8  (calculated-Le Bas method at normal boiling point)
  214.7  (calculated-density)
Dissociation Constant, pKₐ:
  80.20  (Rordorf 1989)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
  16.19  (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_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. Additional data at other temperatures designated * are compiled at the end of this section):
  0.20*  (shake flask-GC/UV, measured range 25–45°C, Richardson & Miller 1960)
  0.20  (Stephen & Stephen 1963)
  0.027  (25–29°C, shake flask-GC/ECD, Park & Bruce 1968)
  0.013*, 0.14*, 0.18* (particle size: 0.01, 0.05 and 5.0µ, shake flask-GC/ECD, Biggar & Riggs 1974)
  0.017  (generator column-GC/ECD, Weil et al. 1974)
  0.027  (Martin & Worthing 1977)
  0.01–0.2  (20–25°C, Wauchope 1978; Willis & McDowell 1982)
  0.013  (Kenaga 1980a, b; Kenaga & Goring 1980; Garten & Trabalka 1983)
  0.027  (27°C, Spencer 1982; Worthing & Walker 1987)
  <0.05  (rm. temp., Hartley & Kidd 1987, Milne 1995)
  0.017–0.18  (Montgomery 1993)
  0.027  (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
  1.06, 0.985  (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
log [C₂H₆/(mol m⁻³)] = −1480/(T/K) + 2.42 (supercooled liquid, linear regression of literature data, 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):
  0.00308  (Porter 1964a)
log (P/mmHg) 2.351 – 2035.35/(T/K); temp range 20–50°C (Porter 1964a)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

0.0008  (Günther & Günther 1971)
0.0031  (20°C, Martin 1972)
0.075   (20°C, Khan 1980)
0.001   (20°C, estimated-relative volatilization rate, Dobbs & Cull 1982)
0.0086* (20°C, extrapolated, gas saturation-GC, measured range 35.5–70°C, Grayson & Fosbracey 1982)
\[ \ln \left( \frac{P}{\text{Pa}} \right) = 32.9 - \frac{11044}{T/\text{K}} \]; temp range 35.5–70°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)
0.023, 0.033 (Pgas by GC-RT correlation, different stationary phases, Bidleman 1984)
0.105  (supercooled liquid Ps, converted from literature Ps with ΔS fus, Bidleman 1984)
0.0092, 0.0071 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = 10.4514 - \frac{4281.065}{T/\text{K}} \]; temp range 25–45°C (gas saturation, Kim 1985)
0.0086 (20°C, Hartley & Kidd 1987)
0.0010 (20°C, Budavari 1989)
0.0081* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
\[ \log \left( \frac{P}{\text{Pa}} \right) = 15.561 - \frac{5262.3}{T/\text{K}} \]; measured range 45–65.2°C (solid, gas saturation-GC, Rordorf 1989)
\[ \log \left( \frac{P}{\text{Pa}} \right) = 12.489 - \frac{4189.8}{T/\text{K}} \]; measured range 105–181°C (liquid, gas saturation-GC, Rordorf 1989)
0.105, 0.0757 (supercooled Ps, converted from literature Ps with different ΔS fus values, Hinckley et al. 1990)
0.0231, 0.0202 (Pgas by GC-RT correlation with different reference standards, Hinckley et al. 1990)
\[ \log \left( \frac{P}{\text{Pa}} \right) = 12.04 - \frac{3924}{T/\text{K}} \] (GC-RT correlation, Hinckley et al. 1990)
0.0031 (20°C, Montgomery 1993)
0.0009 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.061, 0.064 (supercooled liquid Ps; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
\[ \log \left( \frac{P}{\text{Pa}} \right) = -4106/(T/\text{K}) + 12.56 \] (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K OW:

3.01  (Lu & Metcalf 1975)
5.67  (Callahan et al. 1979)
5.66  (calculated, Kenaga 1980a, b)
7.50  (RP-TLC-RT correlation, Lord et al. 1980)
7.40  (extrapolated from RP-TLC, Briggs 1981)
5.66  (shake flask, Geyer et al. 1984)
6.496 ± 0.035 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
5.17–7.40 (Montgomery 1993)
5.74  (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
6.50  (selected, Hansch et al. 1995)
5.74, 5.49, 5.39 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
6.50, 6.24 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K OA at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

8.08* (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
\[ \log K_{OA} = -4.37 + 3709/(T/\text{K}) \]; temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
8.08, 8.26 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

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Bioconcentration Factor, log BCF:

- 0.398 (bioaccumulation factor log BF, adipose tissue in female Albino rats, Quaife et al. 1967)
- 3.56–4.88 (earthworms, Wheatley & Hardman 1968)
- 2.80 (lake bacteria, Leshniovsky et al. 1970)
- 4.36; 4.50; 5.15 (Diptera; Epeneoptera; Cladocera; non-steady-state, Johnson et al. 1971)
- 4.55 (Daphnia magna, wet wt. basis, Johnson et al. 1971)
- 3.56–4.60 (Oedogonium sp., Metcalf et al. 1973)
- 3.50 (Metcalf 1974)
- 3.11 (Anabaena cylindrica, Schaubeger & Wildman 1977)
- 4.03, 3.50 (fish: flow water, static water; Kenaga 1980b)
- 3.85, 1.34 (calculated-S, K_{OW}, Kenaga 1980a)
- 0.431 (average beef fat diet, Kenaga 1980b)
- 4.10 (Chlorella fusca, Geyer et al. 1981)
- 3.59 (golden orfe, Freitag et al. 1982)
- 4.10 (algae, Freitag et al. 1982)
- 4.26 (activated sludge, Freitag et al. 1982, 1984)
- 4.03 (Garten & Trabalka 1983; quoted, Howard 1991)
- 4.13 (clam fat, 60-d expt., Hartley & Johnson 1983)
- 4.09 (Chlorella fusca, Geyer et al. 1984)
- 4.09, 3.44, 4.26 (algae, golden ide, activated sludge, Freitag et al. 1985)
- –1.07 (beef biotransfer factor log B_{st}, correlated-K_{OW} from Radeleff et al. 1952 & Kenaga 1980; Travis & Arms, 1988)
- –1.62 (milk biotransfer factor log B_{st}, correlated-K_{OW} from Saha 1969; Travis Arms 1988)
- –1.67 (vegetation, correlated-K_{OW} from Lichtenstein 1960 & Weisgerber et al. 1974; Travis & Arms, 1988)
- 4.09, 4.79 (algae Chlorella: wet wt basis, dry wt basis, Geyer et al. 2000)
- 4.55, 6.55 (Daphnia: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 3.66, 5.66 (mussel Mytilus edulis: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

- 2.61 (soil, Hamaker & Thompson 1972; quoted, Kenaga 1980a, b; Kenaga & Goring 1980)
- 4.68 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 4.69 (soil, sorption isotherm, converted from K_{OM} multiplied by 1.724, Briggs 1981)
- 4.36 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
- 4.69 (derived from exptl., Meylan et al. 1992)
- 5.02 (calculated-MCI χ, Meylan et al. 1992)
- 6.18 (estimated by QSAR & SPARC, Kollig 1993)
- 2.61, 4.69 (Montgomery 1993)
- 4.69; 4.68 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
- 6.50; 4.70 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization: half-life of a few hours to a few days (Callahan et al. 1979);
calculated t_{1/2} = 68 h from water (Thomas 1982).

Photolysis:
Oxidation: photooxidation t_{1/2} = 0.9–9.1 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: not readily hydrolyzable with t_{1/2} > 4 yr (Callahan et al. 1979);
- first-order t_{1/2} = 760 d, based on a first-order rate constant k = 3.8 × 10^{-5} h^{-1} at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991);
- no disappearance in sealed glass ampoules after two weeks at pH 11 and 85°C (Kollig 1993)
  t_{1/2} = 760 d at pH 7 and 25°C (Montgomery 1993)
t_{1/2} = 760 d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic \( t_{1/2} = 504–14200 \) h, based on unacclimated aerobic river die-away test data and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

rate constant \( k = 0.013 \) d\(^{-1}\) by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic \( t_{1/2} = 24–168 \) h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

\( t_{1/2} = 43–63 \) d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991);

\( t_{1/2} = 21 \) d, \( t_{1/2}(\text{anaerobic}) = 1 \) d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: estimated \( t_{1/2} \sim 35.5 \) min for the vapor phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991);

\( t_{1/2} = 0.9–9.1 \) h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: \( t_{1/2} = 504–14200 \) h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991).

Biodegradation \( t_{1/2}(\text{aerobic}) = 21 \) d, \( t_{1/2}(\text{anaerobic}) = 1 \) d, hydrolysis \( t_{1/2} = 760 \) d at pH 7 in natural waters (Capel & Larson 1995).

Ground water: \( t_{1/2} = 24–28400 \) h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} = 5–10 \) yr persistence in soil (Nash & Woolson 1967);

\( t_{1/2} = 504–14200 \) h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

persistence of 2 yr (Edwards 1973; quoted, Morrill et al. 1982);

more than 24 months of persistence in soil (Wauchope 1978);

estimated first-order \( k = 0.013 \) d\(^{-1}\) with \( t_{1/2} = 53.3 \) d from biodegradation by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent with a \( t_{1/2} = 20–100 \) d (Willis & McDowell 1982; quoted, Howard 1991);

\( t_{1/2} = 43–63 \) d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991);

selected field \( t_{1/2} = 365 \) d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

\( t_{1/2} = 5–9 \) d (Geyer et al. 2000)

Biota:
**TABLE 18.1.1.3.1**

Reported aqueous solubilities and octanol-air partition coefficients of aldrin at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Richardson &amp; Miller 1960</td>
<td>Biggar &amp; Riggs 1974</td>
</tr>
<tr>
<td>shake flask-UV spec.</td>
<td>shake flask-GC</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m–3</th>
<th>t/°C</th>
<th>S/g·m–3</th>
<th>S/g·m–3</th>
<th>S/g·m–3</th>
<th>t/°C</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>particle size</td>
<td>0.01µ</td>
<td>0.05µ</td>
<td>5.0µ</td>
<td>0.0055</td>
<td>0.052</td>
<td>0.105</td>
</tr>
<tr>
<td>25</td>
<td>0.20</td>
<td>15</td>
<td>0.0135</td>
<td>0.140</td>
<td>0.180</td>
<td>10</td>
<td>8.6780</td>
</tr>
<tr>
<td>35</td>
<td>0.39</td>
<td>25</td>
<td>0.030</td>
<td>0.235</td>
<td>0.350</td>
<td>15</td>
<td>8.5419</td>
</tr>
<tr>
<td>45</td>
<td>0.79</td>
<td>35</td>
<td>0.065</td>
<td>0.455</td>
<td>0.600</td>
<td>20</td>
<td>8.2987</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
<td>0.065</td>
<td>0.455</td>
<td>0.600</td>
<td>25</td>
<td>8.0801</td>
</tr>
</tbody>
</table>

$log K_{OA} = A + B/(T/K)$

A: -4.366
B: 3709

enthalpy of phase change
$\Delta H_{OA}/(kJ \ mol^{-1}) = 71.0$

**FIGURE 18.1.1.3.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for aldrin.
FIGURE 18.1.1.3.2 Logarithm of \( K_{OA} \) versus reciprocal temperature for aldrin.

### TABLE 18.1.1.3.2
Reported vapor pressures of aldrin at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Grayson &amp; Fosbracey 1982</th>
<th>Rordorf 1989</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>35.5</td>
<td>0.063</td>
</tr>
<tr>
<td>41.0</td>
<td>0.101</td>
</tr>
<tr>
<td>41.6</td>
<td>0.112</td>
</tr>
<tr>
<td>45.6</td>
<td>0.163</td>
</tr>
<tr>
<td>50.8</td>
<td>0.329</td>
</tr>
<tr>
<td>63.3</td>
<td>1.033</td>
</tr>
<tr>
<td>70.0</td>
<td>2.213</td>
</tr>
<tr>
<td>20</td>
<td>0.0086</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 1a</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>11044</td>
</tr>
<tr>
<td>B</td>
<td>32.9</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 18.1.1.3.3 Logarithm of vapor pressure versus reciprocal temperature for aldrin.
18.1.1.4 Aminocarb

Common Name: Aminocarb
Synonym: A 363, Bay 44646, Bayer 5080, ENT 25784, Matacil, Mitacil
Chemical Name: 4-dimethylamino-<sub>m</sub>-tolyl methylcarbamate, 4-dimethylamino-3-methylphenol methylcarbamate
Uses: nonsystemic, broad-spectrum insecticide used to control the spruce budworm in forests and also as molluscicide.
CAS Registry No: 2032-59-9
Molecular Formula: C<sub>11</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>
Molecular Weight: 208.257
Melting Point (°C): 94 (Lide 2003)
Boiling Point (°C):
Density (g/cm<sup>3</sup> at 20°C):
Molar Volume (cm<sup>3</sup>/mol):
Dissociation Constant, pK<sub>a</sub>:
Enthalpy of Fusion, ∆H<sub>fus</sub> (kJ/mol):
Entropy of Fusion, ∆S<sub>fus</sub> (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S<sub>fus</sub> = 56 J/mol K), F: 0.210 (mp at 94°C)
Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m<sup>3</sup>/mol):
Octanol/Water Partition Coefficient, log K<sub>OW</sub>:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K<sub>OC</sub>:
Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:
Half-Lives in the Environment:

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18.1.1.5 Azinphos-methyl

Common Name: Azinphos-methyl
Synonym: Bay or Bayer 9027, Bay 17147, Carfene, Cotnion, Cotnion methyl, Crysthion 21, DBD, ENT 23233, Gothnion, Gouthion, Gusathion, Metiltriazotion, R 1582
Chemical Name: $O,O$-dimethyl-$S$-[4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate; $O,O$-dimethyl-$S$-[3,4-dihydro-4-keto-1,2,3-benzotriazinyl-3-methyl] dithiophosphate
Uses: nonsystemic insecticide and acaricide for control of insects and pests in blueberry, grape, maize, vegetable, cotton, and citrus crops.
CAS Registry No: 86-50-0
Molecular Formula: $C_{10}H_{12}N_{3}O_{3}PS_{2}$
Molecular Weight: 317.324
Melting Point (°C):
73 (Lide 2003)
Boiling Point (°C):
> 200 (dec., Montgomery 1993)
Density (g/cm$^3$ at 20°C):
1.518 (Tomlin 1994)
1.44 (Milne 1995; Montgomery 1993)
Molar Volume (cm$^3$/mol):
270.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, $pK_a$:
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
96.65 (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
30.96 (DSC method, Plato & Glasgow 1969)
20.5 (Rordorf 1989)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
59 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.338 (mp at 73°C)
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
33 (rm. temp., Spencer 1973; Worthing 1979; Khan 1980; Budavari 1989)
30 (20°C, Melnikov 1971; Spencer 1982)
20.9 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
29 (Hartley & Kidd 1987; Lohninger 1994)
30 (Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
$2.93 \times 10^{-5}$ (20°C, Melnikov 1971)
$0.0510$ (20°C, Khan 1980)
$1.00 \times 10^{-6}$ (20°C, Worthing & Walker 1983)
$1.11 \times 10^{-5}$ (20°C, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)
$3.10 \times 10^{-6}$ (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
$< 0.0010$ (20°C, Hartley & Kidd 1987)
$3.00 \times 10^{-5}$ (20°C, selected, Suntio et al. 1988)
$7.80 \times 10^{-7}$, $3.0 \times 10^{-5}$, $6.90 \times 10^{-4}$, $0.010$, $0.11$ (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_s/P_a) = 14.416 – 6119.2/(T/K); measured range 80.3–145°C (solid, gas saturation-GC, Rordorf 1989)
log (P_s/P_a) = 11.327 – 5048.6/(T/K); measured range 80.3–145°C (liquid, gas saturation-GC, Rordorf 1989)
<1.8 × 10^{-4} (20°C, Worthing & Hance 1991)
1.80 × 10^{-4} (20°C, Tomlin 1994)
2.13 × 10^{-4} (20°C, Montgomery 1993)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
0.0032 (20°C, calculated-P/C, Suntio et al. 1988)
1.52 × 10^{-5} (calculated-P/C, Howard 1991)
3.17 × 10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.99 (Callahan et al. 1979)
2.69 (20°C, shake flask-GC, Bowman & Sans 1983b)
2.75 (Hansch & Leo 1985)
2.43 (HPLC-RT correlation, Moody et al. 1987)
2.69, 2.75 (Montgomery 1993)
2.75 (recommended, Sangster 1993)
2.96 (Tomlin 1994)
2.75 (recommended, Hansch et al. 1995)
2.62 (Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:
1.96 (calculated-S as per Kenaga 1980, this work)
1.86 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
2.61 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
2.28 (Fröbe et al. 1989)
1.30 (selected, USDA 1989; Neary et al. 1993)
2.28 (derived from exp., Meylan et al. 1992)
1.84 (calculated-MCI \chi, Meylan et al. 1992)
2.47–3.53 (Montgomery 1993)
2.95 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.28 (soil, calculated- QSAR MCI \chi, Sabljic et al. 1995)
2.95; 1.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.67, 3.69, 2.73, 2.74, 2.91 (first generation Eurosols ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
2.28; 1.80, 2.04 (soil, quoted exp.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2} = 1.3$ 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: first-order $t_{1/2} = 36.4, 27.9, 7.2$ d in water at pH 8.6 and 6°C, 25°C and 40°C (Heuer et al. 1974; quoted, Howard 1991);
- $t_{1/2} = 27.9$ d at pH 8.6 and 25°C (Montgomery 1993);
- $t_{1/2} = 87$ d at pH 4, $t_{1/2} = 50$ d at pH 7, and $t_{1/2} = 4$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: studies with aquatic water/sediment microorganisms at 5 mg/L and pH 6.7 indicate $t_{1/2} = 3.3$ d in microcosms compared to $t_{1/2} = 2.7$ d in field studies (Portier 1985; quoted, Howard 1991).

Half-Lives in the Environment:

Air: $t_{1/2} = 1.3$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air

Surface water: $t_{1/2} = 415$ d at 6°C, $t_{1/2} = 115$ d at 22°C in darkness for Milli-Q water; $t_{1/2} = 278$ d at 6°C, $t_{1/2} = 42$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 506$ d at 6°C, $t_{1/2} = 35$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 26$ d at 22°C in darkness, $t_{1/2} = 11$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: for dry soil with 2–3% moisture, $t_{1/2} = 484, 88,$ and 32 d at 6, 25, and 40°C, respectively; while for moist soil with 50% moisture content, half-lives were much shorter: 64, 13, and 5 d at 6, 25, and 40°C, respectively (Yaron et al. 1974; quoted, Montgomery 1993);
- selected field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996);
- average $t_{1/2} = 40$ d (Dowd et al. 1993);
- half-life in soil ranges from a few days to many weeks, depending on soil type (Tomlin 1994);
- $t_{1/2} = 10$ d (selected, Halfon et al. 1996).

Biota: average $t_{1/2} = 30$ d in forest (selected, USDA 1989; quoted, Neary et al. 1993).
18.1.1.6 Bendiocarb

![Chemical Structure of Bendiocarb](image)

Common Name: Bendiocarb
Synonym: Bencarbate, Dycarb, Ficam, Garvox, Multamat, Multimet, NC 6897, Niomil, Rotate, Seodox, Tatlo, Turcam
Chemical Name: 2,3-isopropylidenedioxyphenyl methylcarbamate; 2,2-dimethyl-1,3-benzodioxol-4-yl methyl-carbamate
Uses: contact insecticide used to control beetles, wireworms, flies, wasps, and mosquitoes in beets and maize.
CAS Registry No: 22781-23-3
Molecular Formula: C_{11}H_{13}NO_{4}
Molecular Weight: 223.226
Melting Point (°C): 130 (Lide 2003)
Density (g/cm³ at 20°C):
- 1.25 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
- 231.7 (calculated-Le Bas method at normal boiling point)
- 178.6 (calculated-density)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0933 (mp at 130°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 40 (Spencer 1973, 1982)
- 40 (Martin & Worthing 1977; Worthing & Walker 1987; Kenaga 1980;)
- 40 (Lohninger 1994)
- 280 (20°C at pH 7, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
- 6.6 × 10⁻⁴ (Hartley & Kidd 1987)
- 0.00467 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 6.6 × 10⁻⁴ (20°C, Montgomery 1993)
- 0.0046 (quoted, gas saturation-GC, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
- 0.365 (20°C, calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log K_{ow}:
- 5.29 (selected, Dao et al. 1983)
- 1.70 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)
- 1.72 (at pH 6.55, Tomlin 1994)
- 1.70 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
- 1.89 (calculated-S, Kenaga 1980)
Sorption Partition Coefficient, log $K_{oc}$:
- 2.76 (calculated-S, Kenaga 1980)
- 2.76 (Montgomery 1993)
- 2.76 (estimated-chemical structure, Lohninger 1994)
- 1.45–1.60 (Tomlin 1994)
- 1.30, 1.83 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
- Hydrolysis: $t_{1/2} = 4$ d at pH 7 and 25°C (Spencer 1982; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:
- Air:
- Surface water: hydrolysis half-life of 4 d at 25°C and pH 7 under EPA guidelines (Spencer 1982)
- Ground water:
- Sediment:
- Soil: half-life of several days to a few weeks (Hartley & Kidd 1987; quoted, Montgomery 1993); selected field $t_{1/2} = 5.0$ d (Wauchope et al. 1992; Hornsby et al. 1996).
- Biota:
18.1.1.7 Bromophos

Common Name: Bromophos
Synonym: Nexion, S-1942, Omexan, Brofene
Chemical Name: o-4-bromo-2,5-dichlorophenyl O,O-dimethyl phosphorothioate
CAS Registry No: 2104-96-3
Uses: insecticide
Molecular Formula: C₈H₈BrCl₂PS
Molecular Weight: 317.999
Melting Point (°C):
    54 (Lide 2003)
Boiling Point (°C):
    140–142 at 0.01 mmHg (Hartley & Kidd 1987; Worthing & Walker 1987)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ :
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: 0.519 (mp at 54°C)
Water Solubility (g/m³ or mg/L at 25°C):
    40 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)
    0.30 (20°C, shake flask-GC, Bowman & Sans 1979)
    0.652 (20°C, correlated, Bowman & Sans 1983b)
    0.70 (20°C, Worthing & Walker 1987)
Vapor Pressure (Pa at 25°C):
    0.017 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_OW :
    4.88 (shake flask-conc ratio-GC, Bowman & Sans 1983b)
    5.208 ± 0.009 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1991)
    4.88 (recommended, Sangster 1993)
    5.21 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_OA :
Bioconcentration Factor, log BCF or log K_B :
    1.89 (calculated, Kenaga 1980b)
    4.65 ± 0.06 (guppy, calculated on an extractable liquid wt basis, De Bruijn & Hermens 1991)
Sorption Partition Coefficient, log K_OC :
    2.76 (calculated-solubility, Kenaga 1980b)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: hydrolyzed in alkaline media (Worthing 1987).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

\[
k_1 = 0.01307 \text{ mL g}^{-1} \text{ d}^{-1}; k_2 = 0.33 \text{ d}^{-1} \text{ (guppy, De Bruijn & Hermens 1991)}
\]

\[
k_2 = 12 \text{ d}^{-1} \text{ (guppy, calculated-$K_{ow}$, De Bruijn & Hermens 1991)}
\]

Half-Lives in the Environment:
18.1.1.8 Bromophos-ethyl

Common Name: Bromophos-ethyl
Synonym: Nexagan, Filariol
Chemical Name: O-(4-bromo-2,5-dichlorophenyl) O,O-diethyl phosphorothioate
CAS Registry No: 4824-78-6
Uses: insecticide, acaricide
Molecular Formula: C_{10}H_{12}Cl_{2}O_{3}PS
Molecular Weight: 394.049
Melting Point (°C):
  - colorless liquid (Spencer 1982)
Boiling Point (°C):
  - 122–123 (at 0.001 mmHg, Hartley & Kidd 1987; Worthing & Walker 1987)
Density (g/cm³ at 20°C):
  - 1.52–1.55 (Hartley & Kidd 1987; Worthing & Walker 1987)
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ:
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):
  - 2.0 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)
  - 0.44 (20°C, Bowman & Sans 1983b)
  - 0.14 (20°C, Worthing & Walker 1987)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
  - 5.68 (shake flask-concn-ration, Bowman & Sans 1983b)
  - 6.149 ± 0.019 (slow-stirring-GC; De Bruijn et al. 1989)
  - 5.68 (recommended, Sangster 1993)
  - 6.15 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{bi}:
  - 2.62 (fish, calculated, Kenaga 1980b)
Sorption Partition Coefficient, log K_{OC}:
  - 3.48 (soil, calculated-solubility, Kenaga 1980b)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Hydrolysis: at room temp., stable in aqueous suspension at pH < 9, hydrolysed at pH > 9, particularly at higher temperature (Worthing & Walker 1987).

Half-Lives in the Environment:
18.1.1.9 Carbaryl

Chemical Name: carbamic acid, methyl-, 1-naphthyl ester; 1-naphthalenol, methyl carbamate; 1-naphthyl-N-methyl carbamate; 1-naphthalenyl methylcarbamate

Uses: contact insecticide used to control most insects on fruits, vegetables, and ornamentals; also used as growth regulator for fruit thinning of apples.

CAS Registry No: 63-25-2

Molecular Formula: C₁₂H₁₁NO₂

Molecular Weight: 201.221

Melting Point (°C):
145 (Lide 2003)

Boiling Point (°C): dec. on distillation

Density (g/cm³ at 20°C):
0.52–0.61 (Worthing & Hance 1991)

Molar Volume (cm³/mol):
218.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:

Enthalpy of Fusion, ∆Hfus (kJ/mol):
24.27 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion ∆Sfus (J/mol K):

Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.0665 (mp at 145°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

Vapor Pressure (Pa at 25°C or as indicated):

< 0.665 (26°C, Melnikov 1971)
2.80 × 10⁻³ (20°C, Hartley & Graham-Bryce 1980)
< 0.133 (20–25°C, Weber et al. 1980)
1.81 × 10⁻⁴ (Ferreira & Seiber 1981)
7.75 × 10⁻³, 5.39 × 10⁻⁴ (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
Insecticides

< 0.665 (26°C, Hartley & Kidd 1987)
< 0.0053 (Worthing & Hance 1991)
8.77 × 10⁻⁴ (Montgomery 1993)
2.00 × 10⁻⁴ (23.5°C, Tomlin 1994)

Henry’s Law Constant (Pa m³/mol):
0.0013 (calculated-P/C, Suntio et al. 1988;)
4.41 × 10⁻⁴ (calculated-P/C as known LWAPC, Meylan & Howard 1991)
3.18 × 10⁻⁴ (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
1.287 (20°C, calculated-P/C, Montgomery 1993)
< 0.010 (estimated, Mabury & Crosby 1996)
4.48 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
2.36 (shake flask-UV, Fujita et al. 1974)
2.36 (Freed et al. 1976)
2.81 (Hansch & Leo 1979; Rao & Davidson 1980)
2.32 (shake flask-UV, Lord et al. 1980)
2.32 (20°C, shake flask-UV, Briggs 1981)
2.29 (20°C, shake flask-GC, Kanazawa 1981)
2.36 (Lyman et al. 1982; Magee 1991; Trapp & Pussemier 1991)
2.31 (22°C, shake flask-GC, Bowman & Sans 1983b)
2.36 (Hansch & Leo 1985)
2.14 (RP-HPLC-RT correlation, Trapp & Pussemier 1991)
2.63 (HPLC-RT correlation, average, Hu & Leng 1992)
2.31–2.81 (Montgomery 1993)
1.99 (RP-HPLC-RT correlation, Saito et al. 1993)
1.59 (Tomlin 1994)
2.36 (recommended, Hansch et al. 1995)
2.24 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log \( BCF \):
< 0.0 (fish in static water, Metcalf & Sanborn 1975; Freed et al. 1976)
1.89 (calculated-S, Kenaga 1980)
1.08 (calculated-\( K_{oc} \), Kenaga 1980)
1.64 (earthworm, Lord et al. 1980)
0.95 (\( Pseudorasbora parva \), Kanazawa 1981)
1.86 (algae, Freitag et al. 1982)
1.53 (golden orfe, Freitag et al. 1982)
1.95 (activated sludge, Freitag et al. 1982, 1984)
0.954 (topmouth gudgeon, Kanazawa 1983)
1.45 (golden ide, Freitag et al. 1984)
1.85, 1.48, 1.95 (algae, golden ide, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log \( K_{oc} \):
2.36 (soil, Leenheer & Atrichs 1971; LaFleur 1976)
2.36 (Kenaga 1980; Kenaga & Goring 1978)
2.76 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.49 (average of 3 soils, McCall et al. 1980)
2.49 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.02 (soil slurry/shake flask-UV method, converted form reported as log \( K_{om} \) of 1.78, Briggs. 1981)
3.04, 2.50, 2.42 (estimated-S, calculated-S and mp, estimated-\( K_{om} \), Karickhoff 1981)
2.76, 2.66 (estimated-S, $K_{OM}$, Lyman 1982)
2.59 (soil slurry method, Swann et al. 1983)
2.57 (reverse phase HPLC-RT correlation, Swann et al. 1983)
2.14 (calculated-MCI $\chi$, Gerstl & Helling 1987)
2.36 (soil, screening model calculations, Jury et al. 1987b)
2.23 (calculated-MCI $\chi$, Bahnick & Doucette 1988)
2.30 (RP-HPLC-$k'$ correlation, cyanopropyl column, Hodson & Williams 1988)
2.04 (estimated as log $K_{OM}$, Magee 1991)
2.30 (soil, Dowd et al. 1993)
2.02–2.59 (Montgomery 1993)
2.71 (estimated-chemical structure, Lohninger 1994)
2.40 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
2.21, 2.39 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.49–2.62 (sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

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

**Vaporization:** $t_{1/2} = 3000$ d estimated from Henry’s law constant for a body of water 1 m deep, flowing at 1 m/s and with a wind speed of 3 m/s (Howard 1991).

**Photolysis:** $t_{1/2} = 6.6$ d for a mid-summer day at latitude 40°, photolysis is about 4 times faster than in the winter months (Wolfe et al. 1978)

$$t_{1/2}(air) = 52–200$ h in the atmosphere, based on aqueous photolysis data; $t_{1/2}(aq.) = 52–200$ h, based on reported photolysis half-life for summer and winter sunlight at 40°N (Howard et al. 1991)

$$k(aq.) = 6.4 \times 10^{-4}$ h$^{-1}$ (Armburst 2000)

$$k(aq.) = (5.6 \pm 0.3) \times 10^{-5}$ s$^{-1}$ in the presence of UV light, a 30 ppm carbaryl solution at 298 K; in the presence of silver-doped zeolite Y catalyst with 2.42% Ag by weight, the photodecomposition rate becomes 80 times faster. The addition of Suwannee River natural organic matter had a minimal effect on this system, increases or decreases the catalytic photodecomposition rate by a factor of 3 at most (Kanan et al. 2003).

**Oxidation:** photooxidation $t_{1/2} = 4.5–7.4$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$$k_{OH}(aq.) = 3.40 \times 10^{9}$ M$^{-1}$ s$^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies and the field dissipation $t_{1/2} = 8.8$ h (Mabury & Crosby 1996).

**Hydrolysis:** $k(alkaline) = (5.02 \pm 0.03)$ M$^{-1}$ h$^{-1}$ with $t_{1/2} = 1500$ d at pH 5, $t_{1/2} = 15$ d at pH 7 and $t_{1/2} = 0.15$ d at pH 9 and 28°C (Wolfe et al. 1978)

$$t_{1/2} = 312$ h, based on base rate constant at pH 7 and 25°C (Howard et al. 1991)

$$t_{1/2} = 1500$ d at pH 5, $t_{1/2} = 15$ d at pH 7, and $t_{1/2} = 0.15$ d at pH 9 at 27°C (Montgomery 1993)

$$t_{1/2} = 12$ d at pH 7 and $t_{1/2} = 3.2$ h at pH 9 (Tomlin 1994)

$$k = 0.066$ d$^{-1}$ at pH 7, $k = 5.2$ d$^{-1}$ at pH 9; dissipation by hydrolysis from a simulated aquatic system after 30 d: 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6; 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7; and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armburst 2000)

**Biodegradation:**

$t_{1/2}(aerobic) = 40–720$ h, based on unacclimated aerobic river die-away test data and freshwater grab sample data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991)

$t_{1/2} > 3 \times 10^4$ d, assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b)

$$k(aq.) = 2.4 \times 10^{-10}$ mL cell$^{-1}$ d$^{-1}$ in aquatic system (Scow 1982)

$$t_{1/2}(anaerobic) = 160–2880$ h, based on unacclimated aerobic biodegradation (Howard et al. 1991)

$$t_{1/2}(aerobic) = 1.7$ d, $t_{1/2}(anaerobic) = 6.7$ d in natural waters (Capel & Larson 1995)

$k(aerobic) = 1.70 \times 10^{-3}$ h$^{-1}$ (Armburst 2000).

**Biotransformation:**

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

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Half-Lives or Fate Rate Constants in the Environment:

Air: \( t_{\text{1/2}} = 12.6 \text{ h} \), based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Howard 1991);

\( t_{\text{1/2}} = 4.5–7.4 \text{ h} \), based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).

Surface water: hydrolysis \( t_{\text{1/2}} = 1500 \text{ d} \) at pH 5, \( t_{\text{1/2}} = 15 \text{ d} \) at pH 7 and \( t_{\text{1/2}} = 0.15 \text{ d} \) at pH 9; direct photolysis \( t_{\text{1/2}} = 6.6 \text{ d} \); and biolysis \( t_{\text{1/2}} > 3 \times 10^4 \text{ d} \) assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b);

18–20% recovered from pond water after 42 d, 37–42% recovered after 50 d from creek water (Szeto et al. 1979)

\( t_{\text{1/2}} = 3.2–200 \text{ h} \), based on aqueous hydrolysis half-life at pH 9 and 28°C and photolysis half-life for winter sunlight at 40°N (Howard et al. 1991)

Biodegradation \( t_{\text{1/2}} \) (aerobic) = 1.7 d, \( t_{\text{1/2}} \) (anaerobic) = 6.7 d, hydrolysis \( t_{\text{1/2}} = 1500 \text{ d} \) at pH 2, \( t_{\text{1/2}} = 13 \text{ d} \) at pH 7 and \( t_{\text{1/2}} = 0.00013 \text{ d} \) at pH 12 in natural waters (Capel & Larson 1995)

\( t_{\text{1/2}} = 37 \text{ d} \) at 22°C for Milli-Q water at pH 6.1; \( t_{\text{1/2}} = 31 \text{ d} \) at 6°C; \( t_{\text{1/2}} = 11 \text{ d} \) at 22°C in darkness; \( t_{\text{1/2}} = 9 \text{ d} \) under sunlight conditions for river water at pH 7.3; \( t_{\text{1/2}} = 45 \text{ d} \) at 6°C; \( t_{\text{1/2}} = 2 \text{ d} \) at 22°C in darkness for filtered river water at pH 7.3; \( t_{\text{1/2}} = 22 \text{ d} \) at 6°C; \( t_{\text{1/2}} < 2 \text{ d} \) at 22°C in darkness and \( t_{\text{1/2}} = 13 \text{ d} \) under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

dissipation by hydrolysis from a simulated aquatic system after 30 d, 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6, 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7 and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armbrust 2000).

Ground water: \( t_{\text{1/2}} = 3.2–1440 \text{ h} \), based on aqueous hydrolysis half-life at pH 9 and 28°C, and unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: ~ 55% recovered after 50 d in autoclaved water and sediment samples (Szeto et al. 1979)

first-order degradation \( k = 0.392 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 1.8 \text{ d} \) under aerobic conditions, \( k = 0.005 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 125 \text{ d} \) under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation \( k = 0.141 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 4.9 \text{ d} \) under aerobic conditions, \( k = 0.0009 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 746 \text{ d} \) under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarenko & Gan 2004)

Soil: \( t_{\text{1/2}} = 97–251 \text{ h} \) in dry soil and 4458–688 h in wet or saturated soil (Hautala 1978; quoted, Howard 1991);
persistence of less than one month (Wauchope 1978);

\( t_{\text{1/2}} = 3.2–720 \text{ h} \), based on aqueous hydrolysis half-life at pH 9 and 28°C and unacclimated aerobic biodegradation half-life (Howard et al. 1991);

biodegradation rate constant \( k = 0.037 \text{ d}^{-1} \) in soil by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with \( t_{\text{1/2}} = 20–100 \text{ d} \) (Willis & McDowell 1982);

\( t_{\text{1/2}} = 22 \text{ d} \) from screening model calculations (Jury et al. 1987b);

selected field \( t_{\text{1/2}} = 10 \text{ d} \) (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

\( t_{\text{1/2}} = 8 \text{ d} \) (Pait et al. 1992);

biodegradation \( t_{\text{1/2}} = 7–14 \text{ d} \) in a sandy loam and \( t_{\text{1/2}} = 14–28 \text{ d} \) in a clay loam under aerobic conditions for concn. at 1 ppm (Tomlin 1994);

\( t_{\text{1/2}} = 10 \text{ d} \) (selected, Halfon et al. 1996)

Field dissipation \( t_{\text{1/2}} = 8.8 \text{ h} \) (Mabury & Crosby 1996)

\( t_{\text{1/2}} = 14 \text{ d} \) in an aerobic soil, \( t_{\text{1/2}} = 72 \text{ d} \) in an anaerobic aquatic soil (quoted, Bondarenko & Gan 2004)

Biota: biochemical \( t_{\text{1/2}} = 22 \text{ d} \) from screening model calculations (Jury et al. 1987b).
Common Name: Carbofuran
Synonym: Bay 70143, Curaterr, ENT 27164, Furadan, NIA 10242, Niagara 10242, Yaltox
Chemical Name: 2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate; 2,3-dihydro-2,2-dimethyl-7-benzo-furanyl methylcarbamate
Uses: broad-spectrum systemic insecticide, nematocide and acaricide applied in soil to control insects and nematodes; also to control insects and mites on foliage.
CAS Registry No: 1563-66-2
Molecular Formula: C_{12}H_{15}NO_{3}
Molecular Weight: 221.252
Melting Point (°C):
151 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.18 (Hartley & Kidd 1987; Trotter et al. 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
240.8 (calculated-Le Bas method at normal boiling point)
187.5 (calculated-density)
Dissociation Constant, pKₐ:
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: 0.0580 (mp at 151°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
700 (Spencer 1973, 1982; Khan 1980; Weber et al. 1980)
250 (Caro et al. 1976)
320 (19°C, shake flask-GC, Bowman & Sans 1979, 1983b)
700 (Verschueren 1983; Windholz 1983, Budavari 1989)
480 (generator column-HPLC/RI, Swann et al. 1983)
670 (RP-HPLC-RT correlation, Swann et al. 1983)
700 (Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)
320 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)
375 (30°C, Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
1.12 × 10⁻³ (Knudsen effusion method, Cook 1973)
1.11 × 10⁻³ (Caro et al. 1976; Fuhrmann & Lichtenstein 1980)
8.67 × 10⁻⁴ (20°C, Hartley & Graham-Bryce 1980)
2.70 × 10⁻³ (33°C, Khan 1980)
2.70 × 10⁻⁴ (Thomas 1982)
2.20 × 10⁻³, 1.08 × 10⁻⁴ (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
2.70 × 10⁻³ (33°C, Hartley & Kidd 1987)
8.00 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.10 × 10⁻⁵, 7.20 × 10⁻⁵ (20, 25°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- $3.95 \times 10^{-4}$ (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
- $7.69 \times 10^{-4}$ (Jury et al. 1984)
- $9.42 \times 10^{-6}$ (Jury et al. 1987a, b; Jury & Ghodrati 1989)
- $5.10 \times 10^{-4}$ (calculated-P/C, Suntio et al. 1988)
- $7.69 \times 10^{-4}$ (calculated-P/C, Taylor & Glotfelty 1988)
- < 0.010 (estimated, Mabury & Crosby 1996)
- $5.04 \times 10^{-5}$ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 2.32 (Hansch & Leo 1979, 1985)
- 1.60 (from Dow Chemical data, Kenaga & Goring 1980)
- 2.88 (Belluck & Felsot 1981)
- 2.07 (quoted, Karickhoff 1981)
- 1.60 (calculated, Lyman 1982)
- 1.82 (RP-HPLC-RT correlation, Trapp & Pussemier 1991)
- 1.60–2.32 (Montgomery 1993)
- 1.60 (RP-HPLC-RT correlation, Saito et al. 1993)
- 2.32 (recommended, Sangster 1993)
- 1.52 (20°C, Tomlin 1994)
- 1.23–1.42 (Milne 1995)
- 2.32 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
- 1.00 (estimated-log $K_{ow}$, Neely et al. 1974)
- 1.32 (calculated-S, Kenaga 1980)
- 0.60 ($Triaenodes tardus$, Belluck & Felsot 1981)
- 1.00 (selected, Schnoor & McAvoy 1981; Schnoor 1992)
- 1.53 (calculated-log $K_{ow}$, Lyman et al. 1982; quoted, Howard 1991)
- 1.18 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
- 2.07 ($Tilapia nilotica$, Tejada & Magallona 1985)
- 1.00 ($Pila luzonica$, Tejada & Magallona 1985)
- 2.07 (paddy field fish, Tejada 1995)

Sorption Partition Coefficient, log $K_{oc}$:
- 2.20 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 1.67 (calculated values for 6 samples while high organic carbon >15% were omitted from calculation by Felsot & Wilson 1980)
- 1.78–2.20 (3 soils of org. content 0.68–2.01, McCall et al. 1980)
- 2.02 (average of 3 soils, McCall et al. 1980)
- 1.46 (soil/sediments, Rao & Davidson 1980)
- 2.46; 1.51; 1.68 (estimated-S; estimated-S and mp; estimated-$K_{ow}$, Karickhoff 1981)
- 2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 2.25 (calculated-S, Lyman 1982)
- 1.47 (average of 5 different soils, Rao & Davidson 1982)
- 2.11 (retention times of RP-HPLC-RT correlation, Swann et al. 1983)
- 2.00 (soil slurry/shake flask method, Swann et al. 1983; quoted, Howard 1991)
- 1.45 (soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 1.73 (calculated-Freund isotherm linearized for 12 samples, Sukop & Cogger 1992)
- 0.903 (selected, USDA 1989)
- 1.98–2.32 (Montgomery 1993)
- 1.80, 2.01 (soil, estimated-class specific model, estimated-general model, Gramatica et al. 2000)
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization: initial rate constant \( k = 1.2 \times 10^{-3} \) h\(^{-1} \) and a predicted rate constant \( k = 2.9 \times 10^{-4} \) h\(^{-1} \) from soil with \( t_{1/2} = 2390 \) h (Thomas 1982).

Photolysis: near surface direct sunlight photolysis rate constant \( k = 0.003 \) d\(^{-1} \) with \( t_{1/2} \approx 200 \) d (Schnoor & McAvoy 1981; Schnoor 1992); \( t_{1/2} \approx 2, 6, 12 \) h for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991).

Photodegradation (\( \lambda > 290 \) nm) half-lives in aqueous carbofuran solutions: \( t_{1/2} \approx 50 \) min with \( \text{TiO}_2 \) (160 mg/L) + \( \text{O}_2 \); \( t_{1/2} \approx 40 \) min with \( \text{H}_2\text{O}_2 \) (6 \times 10\(^{-3} \) mg/L); \( t_{1/2} \approx 30 \) min with \( \text{O}_3 \) (10\(^{-3} \) mg/L) and \( t_{1/2} \approx 65 \) h in water/oil suspension. (Mansour et al. 1997)

Oxidation: photooxidation \( t_{1/2} = 4.6 \) h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

\[
k(aq.) = (620 \pm 60) \text{ M}^{-1} \text{s}^{-1}
\]
for direct reaction with ozone in water at pH 3.7 and 21°C, with \( t_{1/2} = 54 \) s at pH 7 (Yao & Haag 1991).

\[
k(aq.) = 7 \times 10^9 \text{ M}^{-1} \text{s}^{-1}
\]
for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao 1992);

\[
k_{\text{OH}}(aq.) = 2.20 \times 10^9 \text{ M}^{-1} \text{s}^{-1}
\]
in irradiated field water both in the laboratory and sunlit rice paddies with field dissipation \( t_{1/2} = 16.3 \) h (Mabury & Crosby 1996).

Hydrolysis: aqueous hydrolysis \( t_{1/2} = 5.1 \) wk at pH 7.0 and at 27°C and \( t_{1/2} = 1.2 \) h at pH 10 (Seiber et al. 1978; quoted, Howard 1991);

alkaline chemical hydrolysis rate constant \( k = 6 \times 10^{-5} \) M\(^{-1} \)·s\(^{-1} \) with \( t_{1/2} > 10,000 \) d (Schnoor & McAvoy 1981; Schnoor 1992);

\( t_{1/2} = 690, 8.2, \) and 1.0 wk in water at 25°C and pH 6.0, 7.0 and 8.0, respectively (Chapman & Cole 1982; quoted, Howard 1991);

hydrolysis rate constants: \( k = (30.6 \pm 0.6) \) L min\(^{-1} \)·mol\(^{-1} \) at 15°C, \( k = (67.0 \pm 0.4) \) L/min·mol at 25°C and \( k = (163 \pm 1.0) \) L min\(^{-1} \)·mol\(^{-1} \) at 35°C (Trotter et al. 1991);

\( t_{1/2} = 170 \) wk at pH 4.5, \( t_{1/2} = 690 \) wk at pH 5–6, \( t_{1/2} = 8.2 \) wk at pH 7 and \( t_{1/2} = 1 \) wk at pH 8.0 at 25°C (Montgomery 1993);

\( t_{1/2} > 1 \) yr at pH 4, \( t_{1/2} = 121 \) d at pH 7, and \( t_{1/2} = 31 \) d at pH 9 at 22°C (Tomlin 1994);

rate constant \( k = 5.0 \times 10^{-3} \) M\(^{-1} \)·h\(^{-1} \) at 24°C; \( t_{1/2} = 737 \) h at pH 7.0, \( t_{1/2} = 93.7 \) h at pH 8.0 and \( t_{1/2} = 1.17 \) h at pH 10.0 in aqueous solutions; \( t_{1/2} = 630 \) d at pH 7, \( t_{1/2} = 133 \) d at pH 8, and \( t_{1/2} = 0.87 \) d at pH 10 in aqueous solutions with montmorillonite suspensions (23.9 g/L); \( t_{1/2} = 937 \) d at pH 7, \( t_{1/2} = 76.2 \) d at pH 8, \( t_{1/2} = 0.98 \) d at pH 10 in aqueous solutions with beidellite suspensions (4.9 g/L); \( t_{1/2} = 889 \) d at pH 7, \( t_{1/2} = 113 \) d at pH 8, \( t_{1/2} = 0.78 \) d at pH 10 in aqueous solutions with illite suspensions (9.2 g/L); and \( t_{1/2} = 753 \) d at pH 7, \( t_{1/2} = 80.6 \) d at pH 8, \( t_{1/2} = 0.91 \) d at pH 10 in aqueous solutions with vermiculite suspensions (8.5 g/L) with an initial carbofuran concentration of 1.0 \times 10^{-4} \text{ M} (Wei et al. 2001).

Biodegradation: rate constants \( k = 0.047 \) d\(^{-1} \) from soil incubation studies and \( k = 0.026 \) d\(^{-1} \) in anaerobic system from flooded soil incubation studies both by die-away test (Rao & Davidson 1980; quoted, Scow 1982); \( t_{1/2} = 40 \) d in 0 to 10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: \( t_{1/2} = 4.6 \) h, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: average \( t_{1/2} = 57 \) h in rice paddy water, but pH dependent, e.g., \( t_{1/2} = 1.2 \) h at pH 10 and \( t_{1/2} = 864 \) h at pH 7; \( t_{1/2} = 48 \) and 55 h for two farm ponds (Seiber et al. 1978);

\( t_{1/2} = 2, 6, 12 \) h for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991); measured rate constant \( k = (620 \pm 60) \text{ M}^{-1} \text{s}^{-1} \) for direct reaction with ozone in water at pH 3.7 and 21°C, with \( t_{1/2} = 54 \) s at pH 7 (Yao & Haag 1991).
Ground water:
Sediment:
Soil: persistence of less than one month (Wauchope 1978);
\[ t_{1/2} = 11–13 \text{ d at pH 6.5, and } t_{1/2} = 60–75 \text{ d for a granular formulation (Ahmad et al. 1979; quoted, Montgomery 1993);} \]
estimated first-order \( t_{1/2} = 15 \text{ d in soil from biodegradation rate constant } k = 0.047 \text{ d}^{-1} \) by die-away test from soil incubation studies and \( t_{1/2} = 26 \text{ d from biodegradation rate constant } k = 0.026 \text{ d}^{-1} \) in anaerobic system from flooded soil incubation studies by die-away test (Rao & Davidson 1980; quoted, Scow 1982); moderately persistent in soils with \( t_{1/2} = 20–100 \text{ d (Willis & McDowell 1982);} \]
\( t_{1/2} = 1–2 \text{ months (Hartley & Kidd 1987; quoted, Montgomery 1993);} \]
\( t_{1/2} = 40 \text{ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);} \]
selected field \( t_{1/2} = 50 \text{ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);} \]
soil \( t_{1/2} = 81 \text{ d (Pait et al. 1992);} \]
\( t_{1/2} = 30 \text{ d for soil depth <5 cm, } t_{1/2} = 60 \text{ d for soil depth 5–20 cm and } t_{1/2} = 120 \text{ d for soil depth > 20 cm (Dowd et al. 1993);} \]
\( t_{1/2} = 60 \text{ d in forest soil (Neary et al. 1993);} \]
\( t_{1/2} = 42.4 \text{ d in loam and } t_{1/2} = 95.5 \text{ d in sand (Behrendt & Brüggemann 1993);} \]
\( t_{1/2} = 30–60 \text{ d in soil (Tomlin 1994) \)
Disappearance rate constants \( k = (1.33–5.16) \times 10^{-2} \text{ h}^{-1} \) and \( k = (0.36–1.13) \times 10^{-2} \text{ h}^{-1} \) in non-sterile soil suspensions; \( k = (1.20–5.07) \times 10^{-2} \text{ h}^{-1} \) in sterile soil suspension at 30°C for 5 Spanish soils. Kinetic profiles in 3 consecutive steps assumed as sorption and fast and slow degradation. Disappearance \( t_{1/2} = 24 \text{ h at 30 and } t_{1/2} = 5 \text{ h at 40°C for all 5 soil suspensions; } t_{1/2} = 48 \text{ h at 30°C and } t_{1/2} = 12 \text{ h at 40°C in Soil 3 (Mora et al. 1996) \)
First order rate constants for photolytic decline in sandy soil: \( k = 1.88 \times 10^{-3} \text{ h}^{-1} \) with \( t_{1/2} = 370 \text{ h irradiated in moisture-maintained soil, } k = 0.86 \times 10^{-3} \text{ h}^{-1} \) with \( t_{1/2} = 800 \text{ h, irradiated in air-dried soil, } k = 1.15 \times 10^{-3} \text{ h}^{-1} \) with \( t_{1/2} = 600 \text{ h in dark control moist sandy soil, but not degraded in the dark control air-dry system. The photolytic } k = 7.31 \times 10^{-4} \text{ h}^{-1} \) with \( t_{1/2} = 950 \text{ h in moist soil and the contribution of moisture to irradiated metabolism } k = 1.02 \times 10^{-3} \text{ h}^{-1} \) with \( t_{1/2} = 680 \text{ h (Graebing & Chib 2004) \)
Biota: biochemical \( t_{1/2} = 40 \text{ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);} \]
\( t_{1/2} = 4 \text{ d in wheat/barley (Behrendt & Brüggemann 1993);} \]
average \( t_{1/2} = 60 \text{ d in the forest (USDA 1989; quoted, Neary et al. 1993) \)
18.1.1.11 Carbophenothion

Common Name: Carbophenothion
Synonym: Carbofenotion, Acaridion, Akaridion, Trithion, Garrathion, Nephocarb, Dagadip
Chemical Name: S-chlorophenylthio methyl O,O-diethyl phosphorothioate
Uses: insecticide/acaricide
CAS Registry No: 786-19-6
Molecular Formula: C₁₁H₁₆ClO₂PS₃
Molecular Weight: 342.866
Melting Point (°C):
- < 25 (Montgomery 1993)
Boiling Point (°C):
- 82 (at 0.01 mmHg, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
Density (g/cm³):
- 1.274 (Spencer 1982)
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH₉₆₃ (kJ/mol):
Entropy of Fusion, ΔS₉₆₃ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
- < 2.0 (Martin 1961; Spencer 1982)
- 0.34 (Gunther et al. 1968; Kenaga 1980b; Kenaga & Goring 1980)
- < 40 (Verschueren 1983)
- 0.63 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
- < 1.0 (room temp., Hartley & Kidd 1987, Worthing & Walker 1987)
- 0.61, 0.63, 0.73 (10, 20, 30°C, Montgomery 1993)
- 0.34 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 0.61, 0.63, 0.73 (10, 20, 30°C, Montgomery 1993)
- 0.34 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 40, < 1 (Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
- 0.40 (Menn et al. 1964)
- 4.13 × 10⁻⁵ (20°C, Eichler 1965)
- 4.07 × 10⁻⁵ (20°C, Melnikov 1971)
- 4.0 × 10⁻⁵ (20°C, Hartley & Graham-Bryce 1980)
- 1.07 (Spencer 1982)
- 7.73 × 10⁻³ (20°C, GC-RT correlation, Kim et al. 1984, Kim 1985)
- 1.07 × 10⁻³ (Hartley & Kidd 1987; Montgomery 1993)
- 1.107 × 10⁻³ (selected, Augustijn-Beckers et al. 1994, Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol):
- 0.046 (20°C, Montgomery 1993)
Octanol/Water Partition Coefficient, log Kₐₘₜₐₜ:
- 4.53 (Callahan et al. 1979)
- 5.12 (shake flask-concn ratio-GC, Bowman & Sans 1983b)
Insecticides

5.66 (shake flask-GC, De Bruijn et al. 1989)
5.50 (recommended, 1993)
5.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:
3.07, 3.63 (calculated-solubility, $K_{ow}$, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:
4.66 (Kenaga & Goring 1980)
3.90 (calculated, Kenaga 1980b)
4.98, 4.72, 3.92, 4.48 (Elkhorn sandy loam at pH 6.0, Hugo gravelly sandy loam at pH 5.5, Sweeney sandy clay loam at pH 6.3 and Tierra clay loam at pH 6.2, Rao & Davidson 1982)
3.56 (calculated-MCI $\chi$, Gerstl & Helling 1987)
3.92–4.98 (Montgomery 1993)
5.10, 4.66, 5.07, 4.76, 5.09, 4.69, 4.90 (mg/L, quoted, Augustijn-Beckers et al. 1994)
4.70 (recommended, soil, Augustijn & Beckers 1994; Hornsby et al. 1996)
4.66 (calculated-MCI $\chi$, Sabljic et al. 1995)
4.47, 4.08 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation: $t_{1/2} \geq 100$ d in soil (Verschueren 1983; quoted, Montgomery 1993). Biodegradation and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

Soil: $t_{1/2} \geq 100$ d (Verschueren 1983; quoted, Montgomery 1993);
field $t_{1/2} = 30$ d (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
18.1.1.12 Carbosulfan

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Common Name</td>
<td>Carbosulfan</td>
</tr>
<tr>
<td>Synonym</td>
<td>Marshal, Advantage, Posse, FMC 35001</td>
</tr>
<tr>
<td>Chemical Name</td>
<td>2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate</td>
</tr>
<tr>
<td>Uses</td>
<td>insecticide/acaricide/nematicide</td>
</tr>
<tr>
<td>CAS Registry No</td>
<td>55285-14-8</td>
</tr>
<tr>
<td>Molecular Formula</td>
<td>C_{20}H_{32}N_{2}O_{3}S</td>
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<tr>
<td>Molecular Weight</td>
<td>380.544</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>viscous brown liquid (Hartley &amp; Kidd 1987)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>124–128 (Tomlin 1994; Milne 1995)</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>1.056 (20°C, Hartley &amp; Kidd 1987; Tomlin 1994; Milne 1995)</td>
</tr>
<tr>
<td>Acid Dissociation Constant, pKₐ:</td>
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</tr>
<tr>
<td>Molar Volume (cm³/mol):</td>
<td></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, F:</td>
<td>1.0</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C):</td>
<td>0.30 (Hartley &amp; Kidd 1987; Tomlin 1994)</td>
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<td></td>
<td>0.03 (Milne 1995)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C):</td>
<td>0.041 × 10⁻³ (Hartley &amp; Kidd 1987, Tomlin 1994)</td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C):</td>
<td></td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log K_{ow}:</td>
<td>3.30 (Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>2.20 (Milne 1995)</td>
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<tr>
<td>Octanol/Air Partition Coefficient, log K_{oa}:</td>
<td></td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF or log K_{bi}:</td>
<td></td>
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<tr>
<td>Sorption Partition Coefficient, log K_{oc}:</td>
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</tr>
<tr>
<td>Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:</td>
<td>Volatilization:</td>
</tr>
<tr>
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<tr>
<td>Hydrolysis: hydrolyzed in aqueous media with t_{1/2} &lt; 1 h in pure water at pH 4; t_{1/2} = 22 h at pH 6, t_{1/2} = 7.6 d at pH 7, t_{1/2} = 14.2 d at pH 8 and t_{1/2} &gt; 58.3 d at pH 9 (Haretly &amp; Kidd 1987; Tomlin 1994)</td>
<td></td>
</tr>
</tbody>
</table>
Biodegradation: in soil, rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2–3$ d (Hartley & Kidd 1987).

Biotransformation:

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

Half-Lives in the Environment:

Air:
Surface water: hydrolyzed in aqueous media with half-lives at 25°C are, $t_{1/2} < 1$ h in pure water at pH 4; $t_{1/2} = 22$ h at pH 6, $t_{1/2} = 7.6$ d at pH 7, $t_{1/2} = 14.2$ d at pH 8 and $t_{1/2} > 58.3$ d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

Ground water:

Sediment:

Soil: rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2–3$ d (Hartley & Kidd 1987).

Biota:
18.1.1.13 Chlordane

Common Name: Chlordane

Synonym: A 1068, Aspon-chlordane, Belt, beta-chlordane, CD-68, Chlorindan, Chlor-Kill, Chlortox, Corodane, Cortilan-neu, Dichlorochlordene, Dowchlor, ENT 9932, ENT 25552, HCS 3260, Kypchlor, M 140, Octachlor, Octaterr, Orthoklor, Shell SD 5532, Synklor, Tat chlor 4, Topichlor, Toxiclor, Velcalol

Chemical Name: 1,2,4,5,6,7,8,8-octachloro-3\textsuperscript{a},4,7,7\textsuperscript{a}-tetrahydro-4,7-methano-1\textsuperscript{H}-indane; 1,2,4,5,6,7,8,8-octa-chloro-3\textsuperscript{a},4,7,7\textsuperscript{a}-tetrahydro-4,7-methanoindane

Uses: nonsystemic insecticide with contact, stomach, and respiratory action and also used as fumigant.

CAS Registry No: 57-74-9 (nonstereospecific chlordane); 5103-71-9 (\textit{cis-} or \textit{\alpha-} isomer); 5103-74-2 (\textit{trans-} or \textit{\beta-} isomer); 5564-34-7 (\textit{\gamma-} isomer); 12789-03-6 (technical grade chlordane)

Molecular Formula: C_{10}H_{6}Cl_{8}

Molecular Weight: 409.779

Melting Point (°C):
- 107–108.8 (\textit{cis}-isomer, Callahan et al. 1979; Howard 1991)
- 103–105 (\textit{trans}-isomer, Callahan et al. 1979; Howard 1991)

Boiling Point (°C):
- 175 (at 2 mmHg, Roark 1951; Callahan et al. 1979; Howard 1991; Montgomery 1993)
- 262, 363, 365 (estimated from structure, Tucker et al. 1983)
- 175 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm\textsuperscript{3} at 20°C):
- 1.59–1.63 (Montgomery 1993)

Molar Volume (cm\textsuperscript{3}/mol):
- 340.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_{a}:

Enthalpy of Vaporization, \Delta\textit{H}_{v} (kJ/mol):
- 77.22, 80.26, 82.92 (mixture, \textit{\alpha-}chlordane, \textit{\beta-}chlordane, Rordorf 1989)

Enthalpy of Fusion, \Delta\textit{H}_{fus} (kJ/mol):
- 28.033 (\textit{cis}-isomer, DSC method, Plato 1972)
- 16.45 (\textit{trans}-isomer, DSC method, Plato 1972)

Entropy of Fusion, \Delta\textit{S}_{fus} (J/mol K):
- 56.4 (Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:
- 0.162 (assuming \Delta\textit{S}_{fus} = 56 J/mol K, Mackay et al. 1986)
- 0.140 (20°C, assuming \Delta\textit{S}_{fus} = 56 J/mol K, Suntio et al. 1988)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C and reported temperature dependence equations):
- 1.850 (generator column-GC/ECD, Weil et al. 1974)
- 0.056 (shake flask-LSC, Sanborn et al. 1976)
- 0.056 (Martin & Worthing 1977)
- 0.10 (Hartley & Kidd 1987; Worthing & Walker 1987, 1991)
- 0.56 (Agency for Toxic Substances and Disease Registry 1988; quoted, Burmaster et al. 1991)
- 0.05 (20°C, selected, Suntio et al. 1988)
- 0.032; 0.009–0.056 (shake flask-LSC; lit. range, Johnson-Logan et al. 1992)
- 1.83 (selected, Yalkowsky & Banerjee 1992)
- 0.056 (Montgomery 1993)
- 0.06 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
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0.127 (calculated-group contribution fragmentation method, Kühne et al. 1995)
0.10 (Tomlin 1994; Milne 1995)
0.061, 0.002 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

\[ \log [S_i/(mol/L)] = -0.880 - 1124/(T/K) \] (liquid, cis-isomer, Passivirta et al. 1999)

\[ \log [S_i/(mol/L)] = -0.880 - 1118/(T/K) \] (liquid, trans-isomer, Passivirta et al. 1999)

0.451, 0.402 (cis-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

0.451, 0.615 (trans-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0013 (Martin 1972, Spencer 1973, 1982)

0.0013 (SRI International 1980; Tucker et al. 1983)

0.00227, 1.6 \times 10^{-5}, 1.3 \times 10^{-5} (estimated-bp, Tucker et al. 1983)

2.9 \times 10^{-3}, 3.86 \times 10^{-3} (cis-, trans-chlordane, 20°C, supercooled liquid P_L, Bidleman et al. 1986)

0.0013 (Hartley & Kidd 1987)

0.0011 (20°C, selected, Suntio et al. 1988)

0.0613, 0.00133 (technical, refined, Worthing & Walker 1987)

0.00293, 0.00040 (cis-isomer, GC-RT correlation, supercooled liquid P_L, solid crystal P_S, Foreman & Bidleman 1987)

0.00387, 0.00052 (trans-isomer, GC-RT correlation, supercooled liquid P_L, solid crystal P_S, Foreman & Bidleman 1987)

0.0013 (Agency for Toxic Substances and Disease Registry 1988)

0.027, 0.31, 2.40, 14.0, 69.0 (25, 50, 70, 100, 125°C, chlordane mixture, gas saturation-GC, Rordorf 1989)

\[ \log (P_i/Pa) = 11.968 - 4033.7/(T/K) \] measured range 70.4–115°C (chlordane mixture, liquid, gas saturation-GC, Rordorf 1989)

0.0080, 0.011, 0.98, 6.70, 36 (α-chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

\[ \log (P_i/Pa) = 12.435 - 4332.5/(T/K) \] measured range 50.1–135°C (α-chlordane, liquid, gas saturation-GC, Rordorf 1989)

0.013, 0.16, 1.40, 9.30, 48 (β-chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

\[ \log (P_i/Pa) = 12.318 - 4235.5/(T/K) \] measured range 50/1–135°C (β-chlordane, liquid, gas saturation-GC, Rordorf 1989)

\[ \log (P_i/Pa) = 13.396 - 4803.6/(T/K) \] measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)

4.5 \times 10^{-3}, 5.1 \times 10^{-3}, 4.8 \times 10^{-3} (cis-chlordane, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)

6.3 \times 10^{-3}, 6.9 \times 10^{-3}, 6.7 \times 10^{-3} (trans-chlordane, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)

\[ \log (P_i/Pa) = 12.04 - 4284/(T/K) \] (cis-chlordane, supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)

\[ \log (P_i/Pa) = 11.95 - 4216/(T/K) \] (trans-chlordane, supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990)

0.0013 (refined grade, Worthing & Hance 1991; Tomlin 1994)

0.0610 (technical grade, Worthing & Hance 1991)

0.00269, 0.00813 (cis-chlordane, supercooled liquid P_L at 20°C, 30°C, calculated from Hinckley et al. 1990; Catham & Bidleman 1992)

0.000133 (20°C, Montgomery 1993)

0.00133 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

4.59 \times 10^{-4} (quoted as mean of cis and trans forms from Howard 1991, Mortimer & Connell 1995)

4.68 \times 10^{-3}, 4.15 \times 10^{-3}, 6.57 \times 10^{-4} (cis-chlordane, supercooled liquid P_L; calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

6.58 \times 10^{-3}, 5.84 \times 10^{-3}, 9.66 \times 10^{-4} (trans-chlordane, supercooled liquid P_L; calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

\[ \log (P_i/Pa) = 14.99 - 5407/(T/K) \] (cis-chlordane, solid, Passivirta et al. 1999)

\[ \log (P_i/Pa) = 14.91 - 5333/(T/K) \] (trans-chlordane, solid, Passivirta et al. 1999)

0.080, 0.0073 (cis-chlordane, supercooled liquid P_L; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):

\[
\log \left( \frac{P_L}{P_a} \right) = -\frac{4238}{(T/K)} + 12.32 \quad \text{(cis-chlordane, supercooled liquid)}
\]

\[
\log \left( \frac{P_L}{P_a} \right) = -\frac{4238}{(T/K)} + 12.32 \quad \text{(trans-chlordane, supercooled liquid)}
\]

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

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

Octanol/Air Partition Coefficient, log \( K_{oa} \) at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:
Insecticides


\[ \log K_{OA} = -8.29 + \frac{5217}{T/K}, \text{ temp range 5–25°C} \] 
\( \text{cis-chlordane, gas saturation-GC, Shoeib & Harner 2002} \)


\[ \log K_{OA} = -8.03 + \frac{5036}{T/K}, \text{ temp range 5–25°C} \] 
\( \text{trans-chlordane, gas saturation-GC, Shoeib & Harner 2002} \)


\[ \log K_{OA} = -5.636 + \frac{4179}{T/K}, \text{ temp range 5–25°C} \] 
\( \text{oxychlordane, gas saturation-GC, Shoeib & Harner 2002} \)

8.91, 8.85 (cis-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

8.86, 8.85 (trans-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.51–3.92; 3.60–3.78; 3.28–3.36; 4.10–4.27 (wet wt. basis 96-h test, eastern oysters; pink shrimp; grass shrimp; pin fish, Parrish et al. 1976)

4.69 (Oedogonium cardiacum, Sanborn et al. 1976)

3.66 (spot fish, 24-h flow system, trans-chlordane, Schimmel et al. 1976)

3.57–4.23 (96 h exposures of trans-chlordane to whole marine fish, Schimmel et al. 1976)

4.11–4.34 (186-d chronic exposures, trans-chlordane to sheephead minnow, Parrish et al. 1978)

3.85–4.46 (exposures trans-chlordane to 28-d old second generation sheephead minnow, Parrish et al. 1978)

4.58 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980; Veith & Kosian 1983)

4.01 (green algae, Glooschenko et al. 1979)

4.06, 3.92 (fish: flowing water, static ecosystem, Kenaga 1980a, b; Kenaga & Goring 1980)

3.50 (calculated-S, Kenaga 1980a)

–0.523 (average beef fat diet, Kenaga 1980b)

2.08, 4.32 (estimated-S, K_{OW}, Bysshe 1982)

3.68, 3.64 (α-, γ-chlordane, clam fat, 60-d expt., Hartley & Johnson 1983)

4.06–4.58 (fish, Bysshe 1987)

5.04–5.88 (earthworms, Gish & Hughes 1982;)

3.57–4.20 mean 4.20; 3.36–4.34 mean 4.34 (α-chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)

33.30–4.18 mean 4.18; 3.26–4.30 mean 4.30 (γ-chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)

4.23, 4.26 (α-, γ-chlordane, rainbow trout, steady-state BCF-concentration ratio., Oliver & Niimi 1985)

4.45, 4.20 (α-, γ-chlordane, rainbow trout, kinetic state BCF-ratio of rate const., Oliver & Niimi 1985)

6.15, 4.88 (α-, γ-chlordane, rainbow trout, Lake Ontario field BCF., Oliver & Niimi 1985)

4.58; 4.33, 4.40 (measured for fathead minnow; calculated-K_{OW} for sheepshead minnows, Zaroogian et al. 1985)

4.58; 3.90, 3.92 (measured for fathead minnow; calculated-K_{OW} for pinfish, Zaroogian et al. 1985)

4.58; 4.33, 4.40 (measured for fathead minnow; calculated-K_{OW} for oyster, Zaroogian et al. 1985)

3.70 (oyster, Hawker & Connell 1986)

6.73, 6.99 (total chlordanes, zooplankton, thick-billed murre, Kawano et al. 1986)

3.78, 4.30 (juvenile and adult sheepshead minnow, 28–129 d exposure, Parrish et al. 1978)

6.0–7.0 (zooplankton and Chum salmon, Kawano et al. 1988)

5.57 (Markwell et al. 1989)

3.52, 2.60 (large mouth bass, clams, 106–127 d exposure, NRC 1974)

3.86 (eastern oyster, 10-d exposure, NRC 1974)

3.74 (white sucker and redhorse, Roberts et al. 1977)

2.03, 2.51, 3.0 (frogs, bluegills, goldfish, Verschueren 1983)

6.73, 7.89, 6.99 (total chlordane: zooplankton, Dall’s porpoise, thick-billed murre, Kawano et al. 1986)

4.58 (estimated-S and K_{OW}, Isnard & Lambert 1988)

–2.13 (beef biotransfer factor log B_{BP}, correlated-K_{OW} from Kenaga 1980, Travis & Arms 1988)

–3.43 (milk biotransfer factor log B_{m}, correlated-K_{OW} from Dorough & Hemken 1973, Travis & Arms 1988)

–1.81 (vegetation, correlated-K_{OW} from Dorough & Pass 1973; Tafuri et al. 1977; Travis & Arms 1988)

3.03 (Hydrilla, Himan & Klaine 1992)

4.01, 3.50; 2.80 (estimated: fish-based, duckweed-based, Himan & Klaine 1992)
3.117, 3.098 (cis-, trans-chlordane, goldfish, Park & Erstfeld 1997)
>4.58, >5.56 (fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.38, 5.20 (Daphnia: wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
4.45, 5.58 (fathead minnow: wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
5.26, 6.31 (Chum salmon, 91% lipid: wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
3.04, 3.74 (alga: wet wt basis, dry wt basis, γ-chlordane, Geyer et al. 2000)
3.04, 3.74 (Daphnia: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
4.21, 5.35 (fathead minnow: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
5.04, 6.18 (chum salmon, 9.2% lipid: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
3.68; 3.67 (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} at 25°C or as indicated:
4.33 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
1.58 (screening model calculations, Jury et al. 1987b)
4.64, 4.09 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
5.50, 5.60 (α-chlordane: field sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
5.40, 5.60 (γ-chlordane, field sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
4.58 (soil, screening model calculations, Jury et al. 1987b, 1990)
4.39, 4.19 (calculated-K_{OW} and solubility, Howard 1991)
4.77, 4.94 (α-chlordane: quoted, calculated-MCI χ, Meylan et al. 1992)
5.45, 4.40–4.86 (Aldrich humic acid, soil, Johnson-Logan et al. 1992)
5.90 (estimated by QSAR and SPARC, Kollig 1993)
4.85–5.57 (Montgomery 1993)
5.15 (soil, calculated-MCI χ, Sabljic et al. 1995)
4.33, 4.42 (log K_{a}, cis-, trans-chlordane, Park & Erstfeld 1997)
5.15; 5.03 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volutilization: the volatilization t_{1/2} ~ 7.3 and 7.9 h for γ- and α- chlordane, respectively, from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982, Howard 1991); and t_{1/2} ~ 18–26, 3.6–5.2, 14.4–20.6 d from a model environmental pond (2 m deep), river (3 m deep) and lake (5 m deep), respectively, (Lyman et al. 1982; Howard 1991); t_{1/2} ~ 43 h from a model river 1-m deep flowing 1 m/s based, on the Henry’s law constant of technical chlordane (Lyman et al. 1982, Howard 1991); measured rate constant k = 0.3 d⁻¹ (Glotfelty et al. 1984; Glotfelty et al. 1989); calculated rate constant k = 1.0 d⁻¹ (Glotfelty et al. 1989).
Photolysis:
Oxidation: t_{1/2} = 5.2–51.7 h in air, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
k_{aq}(aq.) = 8 × 10^4 M⁻¹ s⁻¹ for the reaction (photo-Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 3.3 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
k(aq.) < 0.04–> 300 M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 6.2–6.4 and 19 ± 2°C, with 2 min > t_{1/2} > 10 d at pH 7 (Yao & Haag 1991).
k(aq.) = (6–170) × 10^4 M⁻¹ s⁻¹ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 3.3 and at 24 ± 1°C (Haag & Yao 1992).
Hydrolysis: t_{1/2} > 4 yr (Callahan et al. 1979);
first-order t_{1/2} > 197000 yr, based on base rate constant k = 4.3 × 10⁻³ M⁻¹ h⁻¹ at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991).
t_{1/2} = 7.2 × 10^7 d at pH 7 and t_{1/2} = 670 d at pH 12 in natural waters (Capel & Larson 1995)
Biodegradation: aqueous aerobic t_{1/2} = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991);
k = 0.0024 d⁻¹ with a biodegradation t_{1/2} = 1214 d under field conditions (Rao & Davidson 1980);
aqueous anaerobic $t_{1/2} = 24–168$ h, based on soil and freshwater mud grab sample data for aldrin, dieldrin, 
edrin and heptachlor epoxide (Maule et al. 1987; quoted, Howard et al. 1991);
$t_{1/2} = 100$ d in soil (Jury et al. 1990)
$t_{1/2}$(aerobic) = 240 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)

**Biotransformation:**

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

$k_1 = 340$ d$^{-1}$ ($\alpha$, $\gamma$-chlordane, rainbow trout, Oliver & Niimi 1985)
$k_2 = 1.92$ d$^{-1}$ ($\alpha$-chlordane, rainbow trout, Oliver & Niimi 1985)
$k_2 = 0.021$ d$^{-1}$ ($\gamma$-chlordane, rainbow trout, Oliver & Niimi 19850
$k_2 = 0.0974$ d$^{-1}$ ($\gamma$-chlordane from rats, Dearth & Hites 1991)
$k_2 = 0.1170$ d$^{-1}$ ($\alpha$-chlordane from rats, Dearth & Hites 1991)

**Half-Lives in the Environment:**

**Air:** $t_{1/2} = 5.2–51.7$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995);

atmospheric transformation lifetime was estimated to be >1 d (Kelly et al. 1994);

$\text{t}_{1/2} = \text{in the Great Lake's atmosphere.} 16 \pm 5.7 \text{ yr at Eagle Harbor, } 10 \pm 2.3 \text{ yr at Sleeping Bear Dunes and} 6.8 \pm 0.8 \text{ yr at Sturgeon Point (Buehler et al. 2004).}$

**Surface water:** $t_{1/2} = 5712–33264$ h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995)

measured rate constant $k < 0.04- > 300$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 6.2–6.4 and

19 ± 2°C, with a half-life, 2 min > $t_{1/2} > 10$ d at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}$(aerobic) = 240 d, $t_{1/2}$(anaerobic) = 1 d; hydrolysis $t_{1/2} = 7.2 \times 10^5$ d at pH 7 and $t_{1/2} = 670$ d at pH 12 in natural waters (Capel & Larson 1995)

**Ground water:** $t_{1/2} = 11424–66528$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

**Sediment:** $t_{1/2} = 20000$ h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).

**Soil:** $t_{1/2} \sim 6$ yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 5 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$\text{t}_{1/2} = 5712–33264$ h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995)

rate constant $k = 0.0024$ d$^{-1}$ with a biodegradation $t_{1/2} = 1214$ d under field conditions (Rao & Davidson 1980);

field $t_{1/2} = 9$ d in fallow soil (Glitfloty 1981; quoted, Nash 1983);

persistent with $t_{1/2} > 100$ d (Willis & McDowell 1982);

microagroecosystem $t_{1/2} = 10–13$ d in moist fallow soil (Nash 1983);

$\text{t}_{1/2} = 1$ yr in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$\text{t}_{1/2} = 3500$ d from screening model calculations (Jury et al. 1987b);

$\text{t}_{1/2} > 50$ d when subject to plant uptake via volatilization (Ryan et al. 1988);

degradation $t_{1/2} = 100$ d in soil (Jury et al. 1990);

mean $t_{1/2} = 3.3$ yr under field conditions (Howard 1991);

estimated field $t_{1/2} = 350$ d (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996);

$\text{t}_{1/2} = 1–20$ yr in soil, $\text{t}_{1/2} = 5015$ yr in the environment (Geyer et al. 2000)

$\text{t}_{1/2} = 240$ and $7.2$ yr for control and sludge-amended Luddington soils, respectively, for $cis$-chlordane and

$\text{t}_{1/2} = 12.9$ and $9.2$ yr for control and sludge-amended Luddington soils, respectively, for $trans$-chlordane

(Meijer et al. 2001).

**Biota:** $t_{1/2} = 1$ d for daphnids and $t_{1/2} = 60$ d for fish (Callahan et al. 1979; quoted, Wilcock et al. 1993);

elimination $t_{1/2} \sim 60$ d for $\alpha$-chlordane and $t_{1/2} \sim 33$ d for $\gamma$-chlordane in rainbow trout (Oliver & Niimi 1985);

biochemical $t_{1/2} = 3500$ d from screening model calculations (Jury et al. 1987b);

depuration $t_{1/2} = 7.1$ d for $\gamma$-chlordane, and $t_{1/2} = 5.9$ d for $\alpha$-chlordane (rats, Dearth & Hites 1991);

$\text{t}_{1/2} = 12$ d for elimination from $T. \text{liliana}$ (Wilcock et al. 1993).
### TABLE 18.1.1.13.1
Reported octanol-air partition coefficients of chlordane at various temperatures

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<th>cis-chlordane</th>
<th>trans-chlordane</th>
<th>oxychlordane</th>
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<td>generator column-GC/MS</td>
<td>generator column-GC/MS</td>
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<td>log $K_{OA}$</td>
<td>t/°C log $K_{OA}$</td>
<td>t/°C log $K_{OA}$</td>
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</tbody>
</table>

$log K_{OA} = A + B/(T/K)$

A  -8.289  
B   5127

enthalpy of phase change

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 97.5$

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 96.4$

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 80.0$

### FIGURE 18.1.1.13.1A Logarithm of $K_{OA}$ versus reciprocal temperature for cis-chlordane.
FIGURE 18.1.1.13.1B Logarithm of $K_{OA}$ versus reciprocal temperature for trans-chlordane.

FIGURE 18.1.1.13.1C Logarithm of $K_{OA}$ versus reciprocal temperature for oxychlordane.
18.1.1.14 Chlorfenvinphos

Common Name: Chlorfenvinphos
Synonym: Apachlor, Birlane, Clofenvenfos, GC 4092, Sapecron, SD 7859
Chemical Name: 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate; 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate

Uses: soil application of insecticide to control root flies, root worms and other soil insects in vegetables; foliar application to control Colorado beetles on potatoes; scale insects and mite eggs on citrus fruit; stem borers and leafhoppers on rice, maize and sugar cane; and white flies on cotton; aside from control of mosquito larvae, it is also used as acaricide and animal ectoparasiticide.

CAS Registry No: 470-90-6 (Z)-isomer, 18708-87-7 (E)-isomer or cis-chlorfenvinphos, 18708-86-6 trans-chlorfenvinphos
Molecular Formula: C_{12}H_{14}Cl_{3}O_{4}P
Molecular Weight: 359.569
Melting Point (°C):
-19 (Lide 2003)
Boiling Point (°C):
167–170 (at 0.5 mmHg, Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm³ at 20°C):
1.36 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm³/mol):
321.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
96.34 (Rordorf 1989)
Enthalpy of Fusion, ΔH₉ (kJ/mol):
Entropy of Fusion, ΔS₉ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉ = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
145 (20°C, Melnikov 1971)
145 (20°C, Khan 1980)
146 (20°C, Briggs 1981)
124 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
130 (20°C, selected, Suntio et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00053 (20°C, Khan 1980)
2.7 × 10⁻⁵ (Verschueren 1983)
0.0010 (Hartley & Kidd 1987; Tomlin 1994)
0.00010 (20°C, selected, Suntio et al. 1988)
8.20 × 10⁻⁴, 1.70 × 10⁻³, 0.22, 2.0, 14.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (Pv/Pa) = 13.794 – 5032.8/(T/K); measured range 36.9–129°C (liquid, gas saturation-GC, Rordorf 1989)
0.00053 (20°C, Worthing & Hance 1991)
8.91 × 10⁻⁴, 1.35 × 10⁻³, 0.0038 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)
Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):

- 0.00028 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.00029 (calculated-P/C, this work)
- 0.324 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

\[
\log K_{AW} = 0.173 - 1187/(T/K) \quad \text{(van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 3.23 (shake flask-UV, Lord et al. 1980)
- 3.10 (20°C, shake flask-GC, Briggs 1981)
- 3.81 (shake flask-GC, Bowman & Sans 1983)
- 3.84 (shake flask, Eadsforth & Moser 1983)
- 3.79 (HPLC-RT correlation method, Eadsforth & Moser 1983)
- 3.56 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 3.81 (recommended, Sangster 1993)
- 3.85, 4.22 (Z isomer, (E) isomer, Tomlin 1994)
- 3.10 (recommended, Hansch et al. 1995)
- 3.56 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.57 (calculated-S, Kenaga 1980)
- 2.30 (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

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

- 2.45 (calculated-S, Kenaga 1980)
- 2.47 (soil, sorption isotherm, converted from reported log \( K_{OM} \) of 2.23, Briggs 1981)
- 2.77 (soil, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)
- 2.47 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Hydrolysis: at 38°C: \( t_{1/2} > 700 \) h at pH 1.1 and \( t_{1/2} > 400 \) h at pH 9.1; \( t_{1/2} = 1.28 \) h at pH 13 and 20°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: \( t_{1/2} > 24 \) wk in sterile sandy loam and \( t_{1/2} < 1.0 \) wk in nonsterile sandy loam; \( t_{1/2} > 24 \) wk in sterile organic soil and \( t_{1/2} = 1.0 \) wk in nonsterile organic soil (Miles et al. 1979).
18.1.1.15 Chlorpyrifos

Common Name: Chlorpyrifos
Synonym: Brodan, Chlorpyrifos-ethyl, Detmol UA, Dowco 179, Dursban, ENT 27311, Eradex, Killmaster, Lorsban, NA 2783, OMS 971, Pyrinex
Chemical Name: \( O,O\)-diethyl \( O\)-3,5,6-trichloro-2-pyridyl phosphorothioate; \( O,O\)-diethyl \( O\)-(3,5,6-trichloro-2-pyridinyl) phosphorothioate
Uses: insecticide used to control insects on a wide variety of crops including fruits, vegetables, ornamentals and trees.

CAS Registry No: 2921-88-2
Molecular Formula: \( \text{C}_9\text{H}_{11}\text{Cl}_3\text{NO}_3\text{PS} \)
Molecular Weight: 350.586
Melting Point (°C): 42 (Lide 2003)
Boiling Point (°C):

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):

\[ \begin{align*}
\text{Water Solubility (g/m³ or mg/L at 25°C or as indicated)}: \\
0.40, 0.47 & \quad (23, 25°C, Brust 1966) \\
1.12 & \quad (shake flask-GC, Felsot & Dahm 1979) \\
0.70, 0.73 & \quad (19, 20°C, shake flask-GC, Bowman & Sans 1979) \\
0.30 & \quad (23°C, Kenaga 1980a, b) \\
0.30 & \quad (Dow Chemical Data, Kenaga & Goring 1980) \\
2.00 & \quad (35°C, Khan 1980) \\
2.00 & \quad (20–25°C, Willis & McDowell 1982) \\
0.40 & \quad (Verschuieren 1983) \\
0.73 & \quad (20°C, shake flask-GC, Bowman & Sans 1983a, b) \\
1.07, 0.42 & \quad (generator column, RP-HPLC-RT correlation, Swann et al. 1983) \\
0.30 & \quad (Kanazawa 1989) \\
0.40 & \quad (20–25°C, selected, Wauchop et al. 1992; Hornsby et al. 1996) \\
1.93 & \quad (Racke 1993) \\
0.73, 1.30 & \quad (20°C, 30°C, Montgomery 1993) \\
1.40 & \quad (Tomlin 1994) \\
1.18 & \quad (quoted lit., Armbrust 2000) \\
1.61, 1.94 & \quad (supercooled liquid \( S_L \); literature-derived value LDV, final adjusted value FAV, Muir et al. 2004) \\
\end{align*} \]

\[ \begin{align*}
\text{Vapor Pressure (Pa at 25°C at 25°C or as indicated)}: \\
0.00145 & \quad (20°C, Eichler 1965; Wolfdietrich 1965) \\
0.0025 & \quad (Brust 1966; Neely & Blau 1977) \\
0.0037 & \quad (Hamaker 1975) \\
0.00253 & \quad (Melnikov 1971) \\
0.0104 & \quad (30°C, NIEHS 1975) \\
0.0012 & \quad (20°C, Hartley & Graham-Bryce 1980) \\
\end{align*} \]
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0.00088 (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
0.00052 (20°C, GC-RT with mp correction, Kim et al. 1984; Kim 1985)
0.0025 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
0.0015 (20°C, selected, Suntio et al. 1988)
0.0067 (supercooled liquid P_l, GC-RT correlation method, Hinckley et al. 1990)
0.0022; 0.0040 (liquid P_l, GC-RT correlation; quoted lit., Donovan 1996)
0.0023 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0022 (gradient GC method, Tsuzuki 2000)
2.18 × 10^{-3}; 1.86 × 10^{-3}, 0.00407 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)
0.0038, 0.0031 (supercooled liquid P_l; literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry’s Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):

1.0 (Mackay 1985)
1.75 (20°C, calculated-P/C, Suntio et al. 1988)
0.418 (calculated-P/C, Fendinger & Glotfelty 1990; Fendinger et al. 1990)
7.902 (calculated-P/C, Howard 1991)
4.06 × 10^{-3} (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
0.421 (23°C, quoted, Schomburg et al. 1991)
0.421 (calculated-P/C, Montgomery 1993)
0.317, 0.492 (20°C, distilled water, salt water 33.3l, wetted wall column-GC, Rice et al. 1997b)
log K_{aw} = −1187.0/(T/K) + 0.173; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
log K_{aw} = −916.0/(T/K) − 0.674; temp range 8.3–43.5°C, (salt water solution, 33.3l NaCl, wetted-wall column-GC, Rice et al. 1997b)
0.366, 0.366; 0.390 (20°C, microlayer, subsurface natural water of salinity 171 and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
0.341, 0.390; 0.390 (20°C, microlayer, subsurface natural water of salinity 16l and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
0.317, 0.341; 0.366 (20°C, microlayer, subsurface natural water of salinity 12l, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
0.366, 0.414; 487 (20°C, microlayer, subsurface water of salinity 32l, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
0.340, 0.414, 0.869 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.284, 0.356; 0.738 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.337, 0.424, 0.782 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.294, 0.369; 0.750 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.224, 0.268, 0.674 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)
log K_{aw} = −872/(T/K) − 0.775; temp range 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
log K_{aw} = −633/(T/K) − 1.665; temp range 8.3–43.5°C, (surface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
0.74 (quoted lit., Armbrust 2000)
1.090 (calculated-P/C, this work)
0.472, 0.568 (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

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

5.11 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977, 1979)
4.99 (Kenaga 1980b; Kenaga & Goring 1980)
4.82 (Veith et al. 1979)
4.67, 4.77  (RP-HPLC correlation, McDuffie 1981)
4.96  (22°C, shake flask-GC, Bowman & Sans 1983b)
5.20  (shake flask-GC, Schimmel et al. 1983)
4.77  (HPLC-RT correlation, De Kock & Lord 1987)
5.14  (HPLC-RT correlation, Liu & Qian 1988)
5.267  (shake flask/slow-stirring method, De Bruijn et al. 1989)
4.70  (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.31–5.27  (Montgomery 1993)
4.73  (RP-HPLC, Saito et al. 1993)
3.99  (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
4.96  (recommended, Sangster 1993)
5.25  (shake flask-HPLC, Ankley et al. 1994)
5.27  (recommended, Hansel et al. 1995)
4.96  (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
5.11  (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log $K_{OA}$:
8.75  (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
2.67  (rainbow trout, Neely & Blau 1977; quoted, McLeese et al. 1976)
2.67  (mosquito fish for 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
2.65, 2.51  (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
3.09, 3.04  (calculated-S; calculated-$K_{OC}$, Kenaga 1980a)
–1.70  (average beef fat diet, Kenaga 1980b)
2.67  (mosquito fish for 30-d exposure, Veith et al. 1980)
2.65; 2.38  (quoted explt., calculated-$K_{OW}$, Briggs 1981)
3.54  (estimated-regression from log $K_{OW}$, Lyman et al. 1982)
3.08  (estimated-regression from S, Lyman et al. 1982; quoted, Howard 1991)
3.50  (calculated-$K_{OW}$, Mackay 1982)
2.67  (mosquito fish, Veith & Kosian 1983)
–3.55  (beef biotransfer factor log $B_{b}$, correlated-$K_{OW}$ from Kenaga 1980, Travis & Arms 1988)
–4.73  (milk biotransfer factor log $B_{m}$, correlated-$K_{OW}$ from McKellar et al. 1976, Travis & Arms 1988)
2.67; 2.51  (rainbow trout; mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
4.32  (stickleback, lipid-based lab data, Deneer 1994)
2.68  (Pait et al. 1992)

Sorption Partition Coefficient, log $K_{OC}$:
4.13  (soil, quoted from Dow Chemical Data, Kenaga 1980a, b; Kenaga & Goring 1980)
3.93  (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.78  (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
3.96, 4.87  (estimated-S and mp, Karickhoff 1981)
2.92, 4.43, 4.72  (estimated-$K_{OW}$, Karickhoff 1981)
4.11  (soil, Thomas 1982; quoted, Nash 1988)
3.79, 4.0  (soil slurry method, RP-HPLC, Swann et al. 1983)
1.61  (av. value calculated from Freundlich coeffs. without Baldwin Lake site data, Corwin & Farmer 1984)
3.35  (calculated-MCI $\chi$, Gerstl & Helling 1987)
3.78  (soil, screening model calculations, Jury et al. 1987b)
3.27  (average of 2 soils, Kanazawa 1989)
3.78  (soil, 20–25°C, selected, Wauchope et al. 1992)
3.77–4.13  (Montgomery 1993)
3.93  (average, Racke 1993)
4.37  (selected, Lohninger 1994)
3.70  (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
3.46 (sediment, estimated, Paraiba et al. 1999)
4.00 (quoted lit., Armbrust 2000)
3.70; 3.83, 3.76 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.62, 3.63 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
3.46–4.23 (sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Sorption Partition Coefficient, log $K_{OM}$:
3.42 (Felsot & Dahm 1979)
3.78 (average of 3 soils, McCall et al. 1980)
3.90 (exptl., Briggs 1981)
3.10–4.31 (Mingelgrin & Gerstl 1983)
4.24 (quoted, Karickhoff 1985; Neely & Blau 1985)
4.50 (best estimate at low sediment concn., Karickhoff 1985)
4.13, 3.74 (selected, estimated, Magee 1991)

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

Volatilization: based on Henry’s law constant, $t_{1/2} = 9.0$ d for a model river 1 m deep, flowing 1 m/s with a wind velocity of 3 m/s (Howard 1991);
initial $k = 8.8 \times 10^{-2}$ h$^{-1}$ and predicted $k = 1.3 \times 10^{-3}$ h$^{-1}$ from soil with $t_{1/2} = 533$ h (Thomas 1982);
$t_{1/2} = 0.3–3.2$ d for disappearance from an inert surface at 25°C (Meikle et al. 1983).

Photolysis: $t_{1/2}$ (exptl) = 22 d determined under midday summer sunlight in California (Meikle et al. 1983; quoted, Howard 1991)

$k_p = (2.19 \pm 0.17) \times 10^{-2}$ h$^{-1}$, $2.09 \pm 0.17 \times 10^{-2}$ h$^{-1}$ at different initial solute concentrations in aqueous solution at pH 7.0 and 25°C irradiated with a 450-W Hanovia mercury arc lamp. Under various environmental conditions, the estimated $t_{1/2} = 31$ d at a depth of 0.001 cm, $t_{1/2} = 43$ d at a depth of 1-m pure water, $t_{1/2} = 2.7$ yr at 1-m depth river water for midsummer conditions; $t_{1/2} = 345$ d at a depth of 1-m pure water under midwinter surface conditions, all at pH 2 at 40°N latitude, with average light attenuation (Dilling et al. 1984; quoted, Howard 1991; Montgomery 1993)

Oxidation: photooxidation $t_{1/2} = 6.34$ h for the vapor phase reaction with OH radical in air (Howard 1991).

Hydrolysis:

$t_{1/2} = 53$ d at pH 7.4 and 20°C (NieHS 1975; quoted, Freed et al. 1977, 1979);
$t_{1/2} = 120$ d at pH 6.1 and $t_{1/2} = 53$ d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation for hydrolysis rates determination (Freed et al. 1979; quoted, Montgomery 1993)

$k_{\text{alkaline}} = 0.1$ M$^{-1}$ s$^{-1}$, $k_{\text{neutral}} = 1 \times 10^{-7}$ s$^{-1}$, $10^{-7}$–$10^{-9}$ M in aqueous buffer at 20°C (Harris 1982)

$k = (1.08$–$2.0) \times 10^{-3}$ h$^{-1}$ corresponding to half-lives of 13–27 d at pH 7 buffer solution and 25°C (Dilling et al. 1984)

$t_{1/2} = 78$ d relatively independent of pH 1 to 7 (Macalady & Wolfe 1983; quoted, Howard 1991)

$t_{1/2} = 1.5$ d in water at pH 8 and 25°C (Worthing & Hance 1991; Tomlin 1994)

Hydrolytic $k_{\text{acidic}} < 0.008$ d$^{-1}$ in acidic soils with pH ≤ 7.0, corresponding to $t_{1/2} = 92$–341 d and $k_{\text{alkaline}} = (0.006$–$0.063)$ d$^{-1}$ in alkaline soils corresponding to $t_{1/2} = 11$–200 d in abiotic hydrolysis in 37 different soils with pH 3.8–8.5. (Racke et al. 1996)

$k = 0.0009$ d$^{-1}$ at pH 5, $k = 0.023$ d$^{-1}$ at pH 7, $k = 0.044$ d$^{-1}$ at pH 9; measured hydroxy radical rate constant for chlorpyrifos $1.3 \times 10^{-3}$ M$^{-1}$ h$^{-1}$ (Armbrust 2000).

Biodegradation:

$k = 0.014$ d$^{-1}$ in soil at 28°C (Miles et al. 1979; quoted, Klečka 1985)
$k = 0.008$–$0.025$ d$^{-1}$ in soil at 25°C (Getzin 1981; quoted, Klečka 1985)
$k = (–0.000495$ to $–0.00243)$ h$^{-1}$ in nonsterile sediment and $k = (–0.000562$ to $–0.00151)$ h$^{-1}$ in sterile sediment by shake-tests at Range Point and also $k = (–0.00109$ to $–0.00231)$ h$^{-1}$ in nonsterile water and $k = (–0.00144$ to $–0.00197)$ h$^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988)

$t_{1/2} = 39$–51 d in loamy and clay soils under anaerobic conditions, $t_{1/2} = 150$–200 d in anaerobic pond sediments (Racke 1993)

$k_{\text{aerobic}} = 9.47 \times 10^{-4}$ h$^{-1}$ for exposure analysis (Armbrust 2000).
Biotransformation:

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

- Elimination $t_{1/2} = 3.3$ d in channel catfish (Barron et al. 1991)
- $k_1 = 7000 \pm 2000$ L kg$^{-1}$ d$^{-1}$ (guppy, lipid-based modeling data, Deneer 1993)
- $k_2 = 0.40 \pm 0.11$ d$^{-1}$ (guppy, lipid-based modeling data, Deneer 1993)
- $k_1 = (26 \pm 8.0) \times 10^3$ L kg$^{-1}$ d$^{-1}$ (stickleback, lipid-based lab data, Deneer 1994)
- $k_2 = (1.2 \pm 0.4)$ d$^{-1}$ (stickleback, lipid-based lab data, Deneer 1994).

Half-Lives in the Environment:

Air: $t_{1/2} = 6.34$ h for the vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991);
- Reaction rate $k = 4.77 \times 10^{-4}$ min$^{-1}$ in air (Paraiba et al. 1999).

Surface water: based on Henry’s law constant, volatilization $t_{1/2} \approx 9.0$ d for a model river 1-meter deep, flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);
- Half-lives of a 100 mL pesticide-seawater solution containing 10 g of sediment were: $t_{1/2} < 2.0$ d, indoor at 25°C with 12-h photo-period white fluorescent light, $t_{1/2} = 4.6$ d, outdoor-light (stoppered, Pyrex flasks exposed to ambient sunlight with temperature 22–45°C), $t_{1/2} = 7.1$ d, outdoor-dark (foil-covered flasks) and $t_{1/2} = 24$ d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993)
- $t_{1/2} = 120$ d in water at pH 6.1, 20°C (quoted, Lartiges & Garrigues 1995);
- Reaction rate $k = 3.80 \times 10^{-4}$ min$^{-1}$ in water (Paraiba et al. 1999).

Ground water:

Sediment: $t_{1/2} = 24$ d in 10 g untreated sediment/100 mL of a pesticide-seawater solution and $t_{1/2} > 28$ d in 10 g sterile sediment/100 mL of a pesticide-seawater solution (Schimmel et al. 1983)
- $t_{1/2} = 150$–200 d in anaerobic pond sediments (Racke 1993)
- Reaction rate $k = 2.85 \times 10^{-5}$ min$^{-1}$ in sediment (Paraiba et al. 1999)
- First-order degradation $k = 0.034$ d$^{-1}$ with $t_{1/2} = 20.3$ d under aerobic conditions, $k = 0.003$ d$^{-1}$ with $t_{1/2} = 223$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.029$ d$^{-1}$ with $t_{1/2} = 23.7$ d under aerobic conditions, $k = 0.012$ d$^{-1}$ with $t_{1/2} = 57.6$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2} = 17.0$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 2.5$ wk in nonsterile organic soil (Miles et al. 1979);
- $t_{1/2} = 12$ and 24 wk in a silt loam and clay loam, $t_{1/2} = 24$ wk while in sterilized soils; however, temperature also had noticeable effects on decomposition as $t_{1/2} = 25, 13, 6$ wk for soil samples incubated at 15, 25, and 35°C, respectively (Getzin 1981a; quoted, Montgomery 1993);
- Hydrolysis $t_{1/2} = 8$ d in Sultan silt loam (Getzin 1981b; quoted, Montgomery 1993);
- $t_{1/2} = 80–100$ d slowly degraded in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);
- $t_{1/2} = 63$ d from screening model calculations (Jury 1987b);
- Persists in soil for 60–120 d (Worthing & Hance 1991);
- Selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);
- $t_{1/2} = 30$ d (Pait et al. 1992);

Field dissipation $t_{1/2} = 39–51$ d in loamy and clay soils under anaerobic conditions; and aerobic solid degradation $t_{1/2} = 5–141$ d (Racke 1993)
- $t_{1/2} = 60–120$ d (Tomlin 1994)
- Dissipation $t_{1/2} \leq 7$ d when applied to dry soils or the soil surface ($t_{1/2} = 7–14$ d); and $t_{1/2} = 30–60$ d when incorporated into the soil profile (Racke et al. 1996)

First order rate constants for photolytic decline in sandy soil: $k = 2.91 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 240$ h irradiated in moisture-maintained, $k = 2.06 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 340$ h, irradiated in air-dried $k = 1.67 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 420$ h in dark control moist and $k = 0.99 \times 10^{-3}$ h with $t_{1/2} = 700$ h in dark control air-dried sandy soil from Sauk County, WI. The photolytic $k = 8.43 \times 10^{-4}$ h$^{-1}$ with $t_{1/2} = 820$ h in moist soil, $k = 1.07 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 650$ h in dry soil. The contribution of moisture to irradiated metabolism $k = 1.24 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 560$ h, but for dark control system for $k = 6.78 \times 10^{-4}$ h$^{-1}$ with $t_{1/2} = 1020$ h (Graebing & Chib 2004)

Biota: $t_{1/2} = 335$ h clearance from fish (Neely 1980);
- Biochemical $t_{1/2} = 63$ d from screening model calculations (Jury et al. 1987b);
- Elimination $t_{1/2} = 3.3$ d in channel catfish (Barron et al. 1991)
18.1.1.16 Chlorpyrifos-methyl

Common Name: Chlorpyrifos-methyl
Synonym: Reldan
Chemical Name: O,O-dimethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate
Uses: insecticide
CAS Registry No: 5598-13-0
Molecular Formula: C$_7$H$_7$Cl$_3$NO$_3$PS
Molecular Weight: 322.534
Melting Point (°C): 43 (Lide 2003)
Boiling Point (°C):
Density (g/cm$^3$):
Acid Dissociation Constant, pK$_a$:
Molar Volume (cm$^3$/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: 0.666 (mp at 43°C)

Water Solubility (g/m$^3$ or mg/L at 25°C):
4.76 (20°C, shake flask-GC, Chiou et al. 1977)
0.40 (Spencer 1982)
4.0 (Kenaga 1980a, b, Kenaga & Goring 1980)
3.2 (20°C, shake flask, Bowman & Sans 1983b)
4.0 (24°C, Hartley & Kidd 1987; Tomlin 1994)
4.0 (selected, 20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):
5.63 × 10$^{-3}$ (Spencer 1982, Hartley & Kidd 1987; Tomlin 1994)
5.60 × 10$^{-3}$ (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry’s Law Constant (Pa·m$^3$/mol at 25°C):

Octanol/Water Partition Coefficient, log K$_{ow}$:
4.31 (shake flask-GC, Chiou et al. 1977)
4.17 (Kenaga 1980a; Kenaga & Goring 1980)
3.29, 4.30 (Rao & Davidson 1980)
4.30 (shake flask-concn ratio-GC; Bowman & Sans 1983b)
4.31 (recommended, Sangster 1993)
3.99 (HPLC-RT correlation, Sicbaldi & Finizio 1993)
4.24 (Tomlin 1994)
4.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K$_{oa}$:

Bioconcentration Factor, log BCF or log K$_b$:
1.98 (fish, static water, Kenaga & Goring 1980)
2.45, 2.36 (calculated-solubility, K$_{ow}$, Kenaga 1980b)
1.98 (fish, microcosm conditions, Garten & Trabalka 1983)
Sorption Partition Coefficient, log $K_{OC}$:

- 3.52 (soil, Kenaga 1980a; Kenaga & Goring 1980)
- 3.30 (soil, calculated, Kanga 1980b)
- 3.76 (soil, Sabljic 1987)
- 3.48 (estimated, soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.52 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 3.52; 3.36, 3.49 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constant and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis: undergoes rapid photodecomposition in UV light (Spencer 1982).
- Photooxidation:
- Hydrolysis: relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{1/2} = 3$ d at pH 8 (Tomlin 1994)
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

- Air:
- Surface water: estimated $t_{1/2} \sim 38$ d in buffered water at pH 6 (Spencer 1982);
- relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{1/2} = 3$ d at pH 8 (Tomlin 1994).
- Ground water:
- Sediment:
- Soil: field $t_{1/2} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
- $t_{1/2} = 1.5$ and 33 d depending upon soil type and microbial activity (Tomlin 1994).
- Biota:
18.1.1.17 Crotoxyphos

Common Name: Crotoxyphos
Synonym: Ciodrin, Ciovap, Cyodrin, Cypona EC, Decrotox, Duo-kill, Duravos, ENT 24717, Volfazol
Chemical Name: dimethyl\((E)\)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate
Uses: insecticide
CAS Registry No: 7700-17-6
Molecular Formula: C_{14}H_{19}O_{6}P
Molecular Weight: 314.271
Melting Point (°C): liquid
Boiling Point (°C):
135 (at 0.03 mmHg, Montgomery 1993)
Density (g/cm³ at 20°C):
1.2 (Spencer 1982)
Molar Volume (cm³/mol):
264.1 (calculated-density)
Dissociation Constant, pKₐ:
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):
1000 (Günther et al. 1968)
1000 (Melnikov 1971; Spencer 1973, 1982;)
1000 (Martin & Worthing 1977; Worthing & Walker 1987; Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
0.0019 (20°C, Khan 1980)
0.00187, 0.0052, 0.013 (20, 30, 40°C, Spencer 1982)
0.0019 (20°C, Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.00063 (20–25°C, calculated-P/C, Montgomery 1993)
0.00060 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K\textsubscript{OW}:
3.00 (Callahan et al. 1979)
2.23 (Kenaga 1980)
3.30 (shake flask, Log P Database, Hansch & Leo 1987)
3.30 (selected, Sangster 1993)
3.30 (selected, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.10 (calculated-S as per Kenaga 1980, this work)
Sorption Partition Coefficient, log K\textsubscript{OC}:
2.23 (soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)
2.00, 1.70 (soil, quoted exptl., calculated-MCI \chi and fragment contribution, Meylan et al. 1992)
2.23 (Montgomery 1993)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: biodegradation $t_{1/2} = 7.5$ d at pH 9 and $t_{1/2} = 22.5$ d at pH 2 from river die-away tests (Konrad & Chester 1969; quoted, Scow 1982).
18.1.1.18 Cyhalothrin

Common Name: Cyhalothrin
Synonym: Grenade, cyhalothrine
Chemical Name: \((RS)-\alpha\text{-cyano-3-phenoxybenzyl(Z)-(1RS,3RS)-(2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclo-}
propanecarboxylate
Uses: insecticide
CAS Registry No: 68085-85-8
Molecular Formula: C\(_{23}\)H\(_{19}\)ClF\(_3\)NO\(_3\)
Molecular Weight: 449.850
Melting Point (°C):
yellow to brown viscous oil (technical, Hartley & Kidd 1987; Tomlin 1994)
Boiling Point (°C):
187–190/0.2 mmHg (Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm\(^3\)):
Acid Dissociation Constant, pK\(_a\):
Molar Volume (cm\(^3\)/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):
< 1.0 (Worthing & Walker 1983)
0.003 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
0.004 (20°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
~ 1.0 \times 10^{-6} (20°C, Hartley & Kidd 1987)
0.001 \times 10^{-3} (20°C, Tomlin 1994)
1.90 \times 10^{-5} (40°C, Knudsen effusion method, Goodman 1997)
\log (P/Pa) = 13.47 – 5723/(T/K) (Antoine eq., measured range 45–85°C, Goodman 1997)
1.51 \times 10^{-5} (P\(^3\), GC-RT correlation, Tsuzuki 2001)
Henry’s Law Constant (Pa·m\(^3\)/mol):
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
6.02 (HPLC-RT correlation, Hu & Leng 1992)
6.80 (20°C, Tomlin 1994)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):
Bioconcentration Factor, log BCF or log \(K_{\text{b}}\):
Sorption Partition Coefficient, log \(K_{\text{oc}}\):
Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{\frac{1}{2}}\):
Hydrolysis: slowly hydrolysed in sunlight at pH 7–9, more rapidly at pH >9 (Hartley & Kidd 1987; Tomlin 1994).
Half-Lives in the Environment:
Soil: \(t_{\frac{1}{2}} \sim 4–12\) wks (Hartley & Kidd 1987; Tomlin 1994)
18.1.1.19 Lambda-cyhalothrin

Common Name: lambda-cyhalothrin
Synonym: lambda-cyhalothrin
Chemical Name: equal quantities of (S)-α-cyano-3-phenoxybenzyl(Z)-(1R,3R)-3-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate and (S)-α-cyano-3-phenoxybenzyl(Z)-(1S,3S)-3-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate
Uses: insecticide
CAS Registry No: 91465-08-6
Molecular Formula: C_{23}H_{19}ClF_{3}NO_{3}
Molecular Weight: 449.850
Melting Point (°C):
49.2 (Hartley & Kidd 1987; Tomlin 1994; Lide 2003)
Boiling Point (°C):
1.33 (25°C, Tomlin 1994)
Density (g/cm³):
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.005 (20°C, pH 6.5, Hartley & Kidd 1987)
0.005, 0.004 (pH 6.5 in purified water, pH 5.0 in buffered water Tomlin 1994)
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):
2.0 × 10⁻⁷ (20°C, Hartley & Kidd 1987)
2.0 × 10⁻⁷, 2.0 × 10⁻⁴ (20, 60°C, Tomlin 1994)
7.80 × 10⁻⁴* (40°C, Wollerton & Husband 1988, quoted in Goodman 1997)
1.88 (extrapolated-Antoine eq., Goodman 1997)
Heating (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
7.0 (20°C, Tomlin 1994)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment: $t_{1/2} \approx 20$ d in water-sediment mixture in sunlight (Tomlin 1994).
- Soil: $t_{1/2} \approx 4–12$ wk (Hartley & Kidd 1987; Tomlin 1994)

### Biota:

#### TABLE 18.1.1.19.1

Reported vapor pressures of lambda-cyhalothrin 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>40</td>
<td>$7.8 \times 10^{-6}$</td>
<td>40</td>
<td>$1.9 \times 10^{-3}$</td>
</tr>
<tr>
<td>50</td>
<td>$4.0 \times 10^{-5}$</td>
<td>50</td>
<td>$4.7 \times 10^{-3}$</td>
</tr>
<tr>
<td>60</td>
<td>$1.9 \times 10^{-4}$</td>
<td>60</td>
<td>$1.7 \times 10^{-4}$</td>
</tr>
<tr>
<td>70</td>
<td>$8.2 \times 10^{-4}$</td>
<td>70</td>
<td>$6.5 \times 10^{-4}$</td>
</tr>
<tr>
<td>80</td>
<td>$3.2 \times 10^{-3}$</td>
<td>80</td>
<td>$2.0 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Wollerton & Husband 1988

Goodman 1997

### FIGURE 18.1.1.19.1

Logarithm of vapor pressure versus reciprocal temperature for lambda-cyhalothrin.

**EQUATIONS**

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

REFERENCES

- Wollerton & Husband 1988
- Goodman 1997
- quoted in Goodman 1997

**PARAMETERS**

- eq. 1 $P/Pa$
- A $13.47$
- B $5723$
18.1.1.20 Cypermethrin

Common Name: Cypermethrin
Synonym: Agrothrin, Ambush C, Barricade, CCN 52, Cymbush, Cyperkill, Demon, FMC 30980, Folcord, Imperator, Kafil Super, Polytron, Ripcord, Sherpa, Stocade, Toppel
Chemical Name: cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate; (RS)-\(\alpha\)-cyano-3-phenoxybenzyl(1\(RS\),3\(RS\);1\(RS\),3\(SR\))-3(2,2-dichlorovinyl)-2,2-dimethylcyclcopropane-carboxylate
Uses: nonsystemic insecticide with contact and stomach action to control a wide range of insects in fruits, vegetables, vines, potatoes, cucurbits, capsicums, cereals, maize, soybeans, cotton, coffee, cocoa, rice, pecans, ornamentals and forestry, etc.; also used to control flies in animal houses and mosquitoes, cockroaches, houseflies and other pests in public health.

CAS Registry No: 52315-07-8
Molecular Formula: C\(_{22}\)H\(_{19}\)Cl\(_2\)NO\(_3\)
Molecular Weight: 416.297
Melting Point (°C):
70 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
1.23 (Tomlin 1994)
1.25 (Milne 1995)
Molar Volume (cm\(^3\)/mol):
457.7 (calculated-Le Bas method at normal boiling point)
335.7 (calculated-density)
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: 0.362 (mp at 70°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
0.041 (shake flask-GC, Coats & O’Donnell-Jefferey 1979)
0.005–0.01 (Stephenson 1982)
0.010 (20°C, Hartley & Kidd 1987)
0.01–0.2 (21°C, Worthing & Walker 1987)
0.004 (20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
0.004 (Montgomery 1993)
0.004 (at pH 7, Tomlin 1994)
0.009 (20°C, selected, Siebers & Mattusch 1996)

Vapor Pressure (Pa at 25°C or as indicated):
8.7 \times 10^{-7} (Barlow 1978)
4.3 \times 10^{-7} (gas saturation, Grayson et al. 1982)
<1.3 \times 10^{-5} (Spencer 1982)
5.1 \times 10^{-10} (70°C, Hartley & Kidd 1987)
2.4 \times 10^{-6} (GC-RT correlation, supercooled liquid \(P_L\), Hinckley et al. 1990)
1.9 \times 10^{-7} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.9 \times 10^{-7} (20°C, extrapolated, Montgomery 1993)
2.3 \times 10^{-7} (20°C, Tomlin 1994)
2.75 \times 10^{-6}; 2.4 \times 10^{-6}; 1.86 \times 10^{-6}, 1.15 \times 10^{-6} \text{ (liquid } P_L\text{, GC-RT correlation; quoted lit. values, Donovan 1996)}
2.3 \times 10^{-6} (20°C, selected, Siebers & Mattusch 1996)
3.25 \times 10^{-6} \text{ (solid } P^S\text{, converted from } P_L\text{ by GC-RT correlation, Tsuzuki 2001)}
Henry’s Law Constant (Pa·m³/mol) at 25°C or as indicated:

- 0.0199 (20–25°C, calculated-P/C, Montgomery 1993)
- 0.0194 (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
- 0.080 (selected, Siebers & Mattusch 1996)
- 0.0195 (calculated-P/C, this work)

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

- 4.47 (shake flask-GC, Coats & O’Donnell-Jefferey 1979)
- 5.90 (Schimmel et al. 1983)
- 5.2 ± 0.6 (cis-form, HPLC-RT correlation, Muir et al. 1985)
- 5.0 ± 0.6 (trans-form, HPLC-RT correlation, Muir et al. 1985)
- 6.60 (Montgomery 1993)
- 4.47, 6.0 (quoted, Sangster 1993)
- 6.60 (Tomlin 1994)
- 6.05, 6.05 ($\alpha$-, $\beta$-isomer, Hansch et al. 1995)
- 5.62 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.99 (activated sludge, Freitag et al. 1984)
- 3.52, 2.62, 2.99 (algae, golden ide, activated sludge, Freitag et al. 1985)
- 1.73–2.34 (trans-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
- 1.63–2.39 (trans-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
- 1.49–2.05 (trans-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
- 1.53–2.38 (cis-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
- 1.84–2.59 (cis-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
- 1.68–2.02 (cis-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
- 2.89 (Oncorhynchus mykiss, Muir et al. 1994; quoted, Devillers et al. 1996)
- 2.92 (Oncorhynchus mykiss, Muir et al. 1994; quoted, Devillers et al. 1996)

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

- 2.36 (cis-form, silt, $K_p$ on 24% DOC, Muir et al. 1985)
- 2.57 (cis-form, clay, $K_p$ on 56% DOC, Muir et al. 1985)
- 2.59 (trans-form, silt, $K_p$ on 10% DOC, Muir et al. 1985)
- 4.0–4.53 (Montgomery 1993)
- 5.54 (sediments, Maund et al. 2002)

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

Half-Lives in the Environment:

Air:
- Surface water: $t_{1/2} = 5$ d in river water (Tomlin 1994).

Ground water:

Sediment:
- Soil: estimated field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:
18.1.1.21 DDD

Common Name: DDD
Synonym: dichloro diphenyl dichloroethane; \( p,p'-\text{DDD} \); Dilene; ENT 4225; ME 1700; NCI-C00475; Rhothane; \( p,p'-\text{TDE} \); TDE; tetrachlorodiphenylethane

Chemical Name: 1,1-dichloro-2,2-bis(4-chlorophenyl)ethane; 1,1′-(2,2-dichloroethylidene)bis[4-chlorobenzene

Uses: degradation product of DDT used as insecticide.

CAS Registry No: 72-54-8 (\( p,p'-\text{DDD} \) or DDD); 53-10-0 (\( o,p'-\text{DDD} \))

Molecular Formula: \( \text{C}_{14}\text{H}_{10}\text{Cl}_{4} \)

Molecular Weight: 321.041

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³ at 20°C):
312.6 (calculated-LeBas method at normal boiling point)
246.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Dissociation Constant, \( pK_a \):

Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
30.96 (DSC method, Plato & Glasgow 1969)
27.313 (Ruelle & Kesselring 1997)

Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
81.17 (Plato & Glasgow 1969; Hinckley et al. 1990)

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \, \text{J/mol K} \), F: 0.148 (mp at 109.5°C)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.002 (shake flask-LSC, Metcalf et al. 1973)
0.005, 0.015, 0.09* (shake flask-GC with particle sizes: 0.01, 0.05, 5.0 micron, Biggar & Riggs 1974)
0.24 (\( p, p'-\text{DDD} \) shake flask-GC, \( o, p'-\text{DDD} \) with particle sizes: 0.05 micron, Biggar & Riggs 1974)
0.060, 0.10, 0.25, 0.315 (shake flask-GC, \( o, p'-\text{DDD} \) at 15, 25, 35, 45°C with particle sizes: 5.0 micron or less, Biggar & Riggs 1974)
0.020 (generator column-GC/ECD, Weil et al. 1974)
0.005 (Martin & Worthing 1977)
0.09, 0.10 (quoted; \( p,p'-, o,p'-\text{DDD} \), Callahan et al. 1979)
0.004 (shake flask-nephelometry, Hollifield 1979)
0.10 (20°C, selected, \( o,p'-\text{DDD} \), Suntio et al. 1988)
0.16 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)
0.020 (20–25°C, selected, Hornsby et al. 1996)
0.050; 0.010, 0.0035 (quoted; predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

\[ \log \left( \frac{S_i}{(\text{mol/L})} \right) = 0.2910 – 1442/(T/K) \] (liquid, Passivirta et al. 1999)

0.90, 0.738 (\( p,p'-\text{DDD} \), supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.52 × 10⁻⁴ (30°C, \( o, p'-\text{DDD} \), gas saturation-vapor density-GC, Spencer & Cliath 1972; Spencer 1975)
1.36 × 10⁻⁴ (30°C, \( p, p'-\text{DDD} \), gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)
1.63 × 10⁻³, 6.24 × 10⁻⁴ (\( P_{\text{GC}} \) by GC-RT correlation, different stationary phases, Bidleman 1984)
4.34 × 10⁻⁴ (supercooled liquid \( P_L \), converted from literature \( P_S \) with \( \Delta S_{\text{ fus}} \) Bidleman 1984)
Insecticides

1.00 × 10⁻⁴ (20°C, selected, Suntio et al. 1988)
2.00 × 10⁻⁴ (20°C, o,p′-, selected, Suntio et al. 1988)
4.35 × 10⁻³, 9.84 × 10⁻³ (supercooled Pₗ, converted from literature Pₛ with different ∆Sₘₛ values, Hinckley et al. 1990)
1.63 × 10⁻³, 1.10 × 10⁻³ (Pₖₐₜ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (Pₒ/Pₛ) = 12.49 – 4622/(T/K) (supercooled liquid, GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
1.33 × 10⁻⁴ (20–25°C, estimated, Hornsby et al. 1996)
9.69 × 10⁻⁴, 1.13 × 10⁻⁴; 9.16 × 10⁻⁵ (p,p´-DDD, supercooled liquid Pₗ, calculated, GC-RT correlation; converted to solid Pₛ with fugacity ratio F, Passivirta et al. 1999)
log (Pₒ/Pₛ) = 16.23 – 6062/(T/K) (solid, p,p´-DDD, Passivirta et al. 1999)
0.00097, 0.0023 (p,p´-DDD, supercooled liquid Pₗ, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
2.18 (calculated-P/C, Yoshida et al. 1983)
0.27 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)
0.64 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
9.00 (calculated-P/C, Ballschmiter & Wittlinger 1991)
0.669 (p,p´-DDD, wetted wall column-GC, Altschuh et al. 1999)
log [H/(Pa m³/mol)] = 12.20 – 3168/(T/K) (p,p´-DDD, Passivirta et al. 1999)
0.67, 0.50 (p,p´-DDD, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log Kₐₜₕ:
5.99 (O’Brien 1975)
6.02 (Ernst 1977)
6.02 (Veith & Morris 1978; Veith et al. 1979)
5.69 (Hansch & Leo 1979)
5.99, 6.08 (p,p´-, o,p´-DDD, Callahan et al. 1979)
6.00 (Kenaga & Goring 1980)
5.19 (RP-HPLC-RT correlation, Chin et al. 1986)
5.00 (RP-HPLC-RT correlation, De Kock & Lord 1987)
6.217 ± 0.031 (p,p´-DDD, shake flask/slow-stirring method, De Bruijn et al. 1989)
6.02 (recommended, Sangster 1993)
4.82 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
6.22 (recommended, Hansch et al. 1995)
4.87 (o,p´-, RP-HPLC-RT correlation, Finizio et al. 1997)
6.02 (p,p´-DDD, calculated, Passivirta et al. 1999)
6.22, 6.33 (p,p´-DDD, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficients, log Kₐₜ₃ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
8.90 (p,p´-DDD, calculated-Kₐₜₕ/Kₐₜ₃, Wania & Mackay 1996)
9.45 (p,p´-DDD, calculated, Finizio et al. 1997)
10.11*, 10.27 (p,p´-DDD, gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
10.10, 10.03 (p,p´-DDD, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
4.92, 3.92 (Gambusia, Physa, Metcalf et al. 1973)
3.96 (mussel, Ernst 1977)
4.72 (fathead minnow, Veith et al. 1979)
4.09 (calculated-S, Kenaga 1980)
4.11 (calculated-S or Kₐₜₕ, Kenaga & Goring 1980)
3.30 (Triaenodes tardus, Belluck & Felsot 1981)
4.34, 4.42 (mussel, oyster; calculated-K_{OW}, Zaroogian et al. 1985)
4.68 (oyster, Zaroogian et al. 1985; quoted, Hawker & Connell 1986)
2.85–4.29 (benthic macroinvertebrates, Reich et al. 1986)
4.81 (calculated-S and K_{OW}, Isnard & Lambert 1988)
–1.90 (beef biotransfer factor log B_{b}, correlated-K_{OW} from Fries et al. 1969, Travis & Arms 1988)
–2.52 (milk biotransfer factor log B_{m}, correlated-K_{OW} from Fries et al. 1969, Travis & Arms 1988)
0.301 (earthworms, quoted, Menzie et al. 1992)
–0.456, –0.745, –0.602 (earthworms, field/lab. estimated, field leaf litter, calculated-modeled, Menzie et al. 1992)
4.68 (calculated-log K_{OW} as per Mackay 1982, this work)

Sorption Partition Coefficient, log K_{OC}:
4.91 (calculated-S, Kenaga 1980)
4.63 (calculated-S or K_{OW}, Kenaga & Goring 1980;)
5.86 (calculated-S, Mill et al. 1980; quoted, Adams 1987)
5.89 (estimated-QSAR & SPARC, Kollig 1993)
5.00 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization: aquatic half-life of a few days to about a month (summarized data, Callahan et al. 1979).
Photolysis: aquatic t_{1/2} > 150 d (summarized data, Callahan et al. 1979).
Oxidation: aquatic t_{1/2} ~ 3 yr (summarized data, Callahan et al. 1979);
photooxidation t_{1/2} = 13.3–133 h in air, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis:
\[ t_{1/2} \approx 570 \text{ d at pH 9 and } t_{1/2} = 190 \text{ yr at pH 5} \] (summarized data, Callahan et al. 1979);
\[ t_{1/2} = 28 \text{ yr at pH 7 and 25°C, calculated from measured neutral and base catalyzed hydrolysis constants of } (2.8 \pm 0.9) \times 10^{-6} \text{ h}^{-1} \text{ and } 5.2 \text{ M}^{-1} \text{ h}^{-1} \] (Ellington et al. 1987, 1988, 1989; quoted, Howard et al. 1991);
rate constant \[ k = 2.5 \times 10^{-2} \text{ yr}^{-1} \text{ at pH 7 and 25°C} \] (Kollig 1993).
Biodegradation: aqueous aerobic t_{1/2} = 2–15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991); aqueous anaerobic t_{1/2} = 70–294 d, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991).

Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
\[ k_1 = 52.9 \text{ h}^{-1}; k_2 = 0.0058 \text{ h}^{-1} \] (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:
Air: t_{1/2} = 17.7–177 h, based on estimated photooxidation half-life in air (Howard et al. 1991).
Surface water: t_{1/2} = 2–15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)
\[ \text{dehydrochlorination rate constant } k = 5.0 \times 10^{-2} \text{ h}^{-1} \text{ with } t_{1/2} = 13.9 \text{ h for } 1.0 \text{ ppm } p,p'-\text{DDD and } k = 0.76 \times 10^{-2} \text{ h}^{-1} \text{ with } t_{1/2} = 96.3 \text{ h for } o,p'-\text{DDD both at } 21 \pm 2°C \text{ and pH 12.8 (in 0.1 N NaOH solution)} \] (Choi & Chen 1976)
\[ \text{estimated } t_{1/2} = 45 \text{ d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)} \]
Ground water: t_{1/2} = 1680–270,000 h, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).
Sediment:
\[ t_{1/2} = 2–15.6 \text{ yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991); estimated field } t_{1/2} \approx 1000 \text{ d (20–25°C, Hornsby et al. 1996)} \]
Biota: t_{1/2} = 119 h in mussel (Ernst 1977).
TABLE 18.1.1.21.1
Reported aqueous solubilities and octanol-air partition coefficients of DDD at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>log $K_{OA}$</th>
<th>p,p'-DDD</th>
<th>o,p-DDD</th>
<th>p,p'-DDD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>shake flask-GC</td>
<td>shake flask-GC</td>
<td>generator column-GC/MS</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>
<td>t/°C</td>
</tr>
<tr>
<td>particle size</td>
<td></td>
<td></td>
<td></td>
<td>particle size</td>
</tr>
<tr>
<td>15</td>
<td>0.01µ</td>
<td>–</td>
<td>0.050</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>0.005</td>
<td>0.015</td>
<td>0.090</td>
<td>25</td>
</tr>
<tr>
<td>35</td>
<td>–</td>
<td>–</td>
<td>0.150</td>
<td>35</td>
</tr>
<tr>
<td>45</td>
<td>–</td>
<td>–</td>
<td>0.240</td>
<td>45</td>
</tr>
</tbody>
</table>

$log K_{OA} = A + B/(T/K)$

A = -5.193
B = 4610

enthalpy of phase change
$ΔH_{OA}/(kJ mol⁻¹) = 80.1$

FIGURE 18.1.1.21.1A Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for p,p'-DDD.
FIGURE 18.1.21.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for $o,p'$-DDD.

FIGURE 18.1.21.2 Logarithm of $K_{OA}$ versus reciprocal temperature for $p,p'$-DDD.
18.1.1.22 DDE

Common Name: DDE \((p,p'-\text{DDE}; o,p'-\text{DDE})\)
Synonym: 4,4'-DDE, DDE; 2,4-DDE
Chemical Name: 1,1-dichloro-2,2-bis(p-chlorophenyl)ethylene
CAS Registry No: 72-55-9 \((p,p'-\text{DDE})\); 3424-82-6 \((o,p'-\text{DDE})\)
Molecular Formula: \(\text{C}_4\text{H}_8\text{Cl}_4\)
Molecular Weight: 319.0
Melting Point \(\degree\text{C}\): 89 \((\text{Lide 2003})\)
Boiling Point \(\degree\text{C}\): 210
Density (g/cm\(^3\) at 20\(^\circ\text{C}\)): 305.2 \((\text{calculated-Le Bas method at normal boiling point})\)
Molar Volume (cm\(^3\)/mol): 210.2 \((\text{Ruelle & Kesselring 1997; Passivirta et al. 1999})\)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
\(30.543\) \(\text{(o,p'-DDE, DSC method, Plato & Glasgow 1969)}\)
\(24.267\) \(\text{(p,p'-DDE, DSC method, Plato & Glasgow 1969)}\)
Entropy of fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
67.0 \((\text{Hinckley et al. 1990; Passivirta et al. 1999})\)
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F: 0.236 (mp at 89°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):
\(p,p'-\text{DDE}\)
0.0013 \((\text{shake flask-LSC, Metcalf et al. 1973, 1975})\)
0.12* \((\text{shake flask-GC for particles 5} \mu\text{- or less, measured range 15–45°C, Biggar & Riggs 1974})\)
0.014 \((\text{generator column-GC/ECD, Weil et al. 1974})\)
0.040 \((20\degree\text{C}, \text{shake flask-GC, Chiou et al. 1977; Freed et al. 1977})\)
0.065 \((\text{shake flask-nephelometry, Hollifield 1979})\)
0.0079 \((\text{Kenaga & Goring 1980})\)
0.0017 \((30\degree\text{C}, \text{semimicro gas-saturation method, Westcott et al. 1981})\)
0.0011, 0.006 \((\text{generator column-GC, HPLC-RT correlation, Swann et al. 1983})\)
\(\log [\text{S}_i/(\text{mol/L})] = 0.173 – 1263/(\text{T/K})\) (liquid, Passivirta et al. 1999)
0.00012 ± 0.00010 \((\text{mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001})\)
0.258, 0.252 \((\text{supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005})\)
\(o,p'-\text{DDE}\)
0.140 \((\text{shake flask-GC for particles 5} \mu\text{- or less, Biggar & Riggs 1974})\)
0.0013 \((\text{Zepp et al. 1978})\)
0.10 \((\text{selected, Suntio et al. 1988; Hornsby et al. 1996})\)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
\(p,p'-\text{DDE}\)
\(8.65 \times 10^{-4}\) \((30\degree\text{C}, \text{gas saturation-vapor density-GC, Spencer & Cliath 1972})\)
\(9.87 \times 10^{-4}\) \((\text{GC-RT correlation, Westcott & Bidleman 1981})\)
\(1.73 \times 10^{-4}\) \((30\degree\text{C}, \text{gas saturation-GC, Westcott et al. 1981})\)
\(8.66 \times 10^{-4}\) \((\text{selected, Yoshida et al. 1983})\)
\(2.70 \times 10^{-3}\), \(2.09 \times 10^{-3}\) \((P_{\text{GC}} \text{by GC-RT correlation, different stationary phases, Bidleman 1984})\)
\(2.55 \times 10^{-3}\) \((\text{supercooled liquid} P_1, \text{converted from literature} P_3 \text{with } \Delta S_{\text{fus}} \text{Bidleman 1984})\)
1.73 × 10⁻³ (20°C, supercooled liquid value, Bidleman et al. 1986)
7.50 × 10⁻⁵ (10°C, estimated, McLachlin et al. 1990)
0.00225, 0.00334 (supercooled liquid values, GC-RT correlation, Hinckley et al. 1990)
2.33 × 10⁻³, 3.34 × 10⁻³ (supercooled P₈, converted from literature P₈ with different ∆Sᶠus values, Hinckley et al. 1990)
2.58 × 10⁻³, 1.87 × 10⁻³ (P₈ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P₈/Pa) = 12.79 – 4554/(T/K) (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
5.13 × 10⁻⁴, 1.82 × 10⁻³ (supercooled liquid values at 10°C, 20°C, Cotham & Bidleman 1992)
4.36 × 10⁻³ (supercooled liquid value, quoted, Majewski & Capel 1995)
2.27 × 10⁻³, 2.78 × 10⁻³; 5.45 × 10⁻⁴ (supercooled liquid P₈: calculated; GC-RT correlation; converted to solid P₈ with fugacity ratio F, Passivirta et al. 1999)
log (P₈/Pa) = 16.29 – 5816/(T/K) (solid, Passivirta et al. 1999)
5.13 × 10⁻⁴, 1.82 × 10⁻³ (supercooled liquid P₈: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
27.4 (Levins 1981; quoted, Tucker et al. 1983)
0.78 (estimated-group method per Hine & Mookerjee 1975)
6.89 (calculated-P/C, Mabey et al. 1982)
124 (gas stripping-GC, Atlas et al. 1982)
19.59 (calculated-P/C, Yoshida et al. 1983)
7.95 (calculated-P/C, Suntio et al. 1988)
1.25 (10°C, calculated-P/C, McLachlin et al. 1990)
34.0 (calculated-P/C, Ballischmierer & Wittlinger 1991)
120, 370 (23°C, 7.95 (20°C) (quoted, Iwata et al. 1993)
7.95 (20–25°C, calculated-P/C, Majewski & Capel 1995)
4.214 (p,p′-DDE, wetted wall column-GC, Altschuh et al. 1999)
log (H/(Pa m³/mol)) = 12.62 – 3291/(T/K) (p,p′-DDE, Passivirta et al. 1999)
4.2, 4.2 (p,p-DDE, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log Kₐw:
5.80 (o,p-DDE, O’Brien 1975)
4.28 (correlated, Metcalf et al. 1975)
5.69 (p,p′-DDE, O’Brien 1975)
5.83 (p,p′-DDE, HPLC-RT correlation, Veith et al. 1979a)
5.69 (HPLC-RT correlation, Veith et al. 1979b)
5.77 (Kenaga & Goring 1980)
5.89 (HPLC-RT correlation, McDuffie 1981)
5.63 (RP-HPLC-RT correlation, Swann et al. 1983)
5.89 (estimated-HPLC/MS correlation, Burkhard et al. 1985)
6.51 (HPLC-RT correlation, Webster et al. 1985)
6.29 (RP-HPLC correlation, Chin et al. 1986)
6.09 (RP-HPLC correlation, De Kock & Lord 1987)
6.956 ± 0.011 (p,p′-DDE, shake flask/slow stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)
6.51 (recommended, Sangster 1993)
5.78 (RP-HPLC correlation, Sichaldi & Finizio 1993)
6.96 (recommended, Hansch et al. 1995)
5.43 (o,p′-, RP-HPLC correlation, Finizio et al. 1997)
6.65 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
6.96, 6.93 (p,p′-DDE, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
Insecticides

Octanol/Air Partition coefficient, log $K_{oa}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Log $K_{oa}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.40</td>
<td>($p,p'$-DDE, calculated-$K_{ow}/K_{ow}$, Wania &amp; Mackay 1996)</td>
</tr>
<tr>
<td>9.45</td>
<td>($p,p'$-DDE, calculated, Finizio et al. 1997)</td>
</tr>
</tbody>
</table>

$\log K_{oa} = -7.49 + \frac{5116}{(T/K)}$; temp range: 5–35°C ($p,p'$-DDE, gas saturation-GC, Shoeib & Harner 2002)

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Organism</th>
<th>Log BCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gambusia, Physa</td>
<td>4.44, 4.29 (Metcalf et al. 1973)</td>
</tr>
<tr>
<td>Algae, snail, mosquito, fish</td>
<td>4.05, 4.56, 4.77, 4.08 (Metcalf et al. 1973)</td>
</tr>
<tr>
<td>Fathead minnows</td>
<td>4.71 (Veith et al. 1979; Veith &amp; Kosian 1983)</td>
</tr>
<tr>
<td>Calculated-S or $K_{ow}$</td>
<td>3.80 (Kenaga &amp; Goring 1980)</td>
</tr>
<tr>
<td>Quoted exptl, calculated-$K_{ow}$</td>
<td>4.71, 4.37 (Mackay 1982)</td>
</tr>
<tr>
<td>Microorganism-water</td>
<td>5.95 (Mabey et al. 1982)</td>
</tr>
</tbody>
</table>

Bioaccumulation Factor, log BAF:

<table>
<thead>
<tr>
<th>Organism</th>
<th>Log BAF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rainbow trout</td>
<td>8.35 (Thomann 1989)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Log $K_{oc}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.48 (calculated-S or $K_{ow}$, Kenaga &amp; Goring 1980;)</td>
</tr>
<tr>
<td>6.64 (sediment, calculated-$K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>4.70, 5.17 (quoted, calculated-MCI $\chi$, Sabljic 1984)</td>
</tr>
<tr>
<td>6.00, 5.30 ($p,p'$-DDE, field data of sediment trap material, calculated-$K_{ow}$, Oliver &amp; Charlton 1984)</td>
</tr>
<tr>
<td>3.70 (soil, estimated, Hornsby et al. 1996)</td>
</tr>
<tr>
<td>4.82 (av. lit. value, Gerstl 1990)</td>
</tr>
<tr>
<td>4.82 ($p,p'$-DDE, soil, calculated- MCI $\chi$, Sabljic et al. 1995)</td>
</tr>
<tr>
<td>4.85 ($p,p'$-DDE, soil, estimated-general model, Gramatica et al. 2000)</td>
</tr>
</tbody>
</table>

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

**Volatilization:**

Photolysis: midday $t_{1/2} = 5$ h in hydrocarbon media (Zepp et al. 1976)

$\ t_{1/2} = 1.5$ d under sunlight in water (Mansour & Feicht 1994).

**Oxidation:**

Hydrolysis: the first-order rate constant $k = 1.4 \times 10^{-9}$ M$^{-1}$ s$^{-1}$ and the hydrolytic $t_{1/2} > 120$ yr in water at 27°C (Wolfe et al. 1977);

hydrolytic $t_{1/2} = 120$ yr at pH 7 and 25°C of 120 yr and a rate constant $k = 6.6 \times 10^{-7}$ h$^{-1}$ (Callahan et al. 1979, Mabey et al. 1982).

**Biodegradation:**

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

$k_1 = 170.0$ d$^{-1}$; $k_2 = 0.021$ d$^{-1}$ ($p,p'$-DDE, rainbow trout, Oliver & Niimi 1985)
$k_2 = 0.950 \text{ yr}^{-1}$ (Larus argentatus, Norstrom et al. 1986)
$k_1 = 20800 \text{ d}^{-1}$; $k_2 = 0.020 \text{ d}^{-1}$ (Oligochaetes, Connell et al. 1988)
$k_2 = 0.0004 \text{ h}^{-1}$ (azalea leaves, Paterson et al. 1991)
$k_2 = 0.0030 \text{ h}^{-1}$ (midge C. riparius, water only system, Lydy et al. 1992)
$k_2 = 0.0046 \text{ h}^{-1}$ (midge C. riparius, screened, Lydy et al. 1992)
$k_2 = 0.0080 \text{ h}^{-1}$ (midge C. riparius, 3% organic carbon, Lydy et al. 1992)
$k_2 = 0.0046 \text{ h}^{-1}$ (midge C. riparius, 15% organic carbon, Lydy et al. 1992)

Half-Lives in the Environment:
Air: atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
Surface water: midday $t_{1/2} = 5 \text{ h}$ in hydrocarbon media (Zepp et al. 1976)
hydrolytic $t_{1/2} > 120 \text{ yr}$ in water at 27°C (Wolfe et al. 1977);
estimated $t_{1/2} = 690 \text{ d}$ in surface waters in case of first order reduction process, and estimated $t_{1/2} > 300 \text{ d}$ in lakes in the Netherlands (Zoeteman et al. 1980);
photolysis $t_{1/2} = 1.5 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).
Ground water:
Sediment:
Soil: field $t_{1/2} = 1000 \text{ d}$ (estimated, Hornsby et al. 1996);
$t_{1/2} > 20 \text{ yr}$, very persistent (Geyer et al. 2000)
$t_{1/2} = 40.9$ and 17.2 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
Biota: elimination $t_{1/2} = 340 \text{ d}$ ($p,p'$-DDE, rainbow trout, Oliver & Niimi 1985);
$t_{1/2} = 264 \text{ d}$ in herring gulls compared to literature average $t_{1/2} = 300 \text{ d}$ for birds (Norstrom et al. 1986);
elimination $t_{1/2} = 2230 \text{ h}$ (Azalea leaves, Bacci & Gaggi 1987);
$t_{1/2} = 231 \text{ h}$ in the midge (Chironomus riparius) under varying sediment conditions (water only system with no sediment), $t_{1/2} = 150 \text{ h}$ (midge screened from the sediment), $t_{1/2} = 87 \text{ h}$ (midge screened from 3% organic carbon sediment), $t_{1/2} = 99 \text{ h}$ (midge screened from 3% organic carbon sediment) (Lydy et al. 1992).

### TABLE 18.1.1.22.1
**Reported aqueous solubilities of DDE at various temperatures**

<table>
<thead>
<tr>
<th></th>
<th>$p,p'$-DDE</th>
<th>$o,p'$-DDE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Biggar &amp; Riggs 1974</td>
<td>Biggar &amp; Riggs 1974</td>
</tr>
<tr>
<td></td>
<td>shake flask-GC</td>
<td>shake flask-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
</tr>
<tr>
<td>particle size</td>
<td>0.01µ</td>
<td>0.05µ</td>
</tr>
<tr>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.010</td>
<td>0.040</td>
</tr>
<tr>
<td>35</td>
<td>0.235</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>0.450</td>
<td></td>
</tr>
</tbody>
</table>
**FIGURE 18.1.1.22.1A** Logarithm of mole fraction solubility (ln $x$) versus reciprocal temperature for $p,p'$-DDE.

**FIGURE 18.1.1.22.1B** Logarithm of mole fraction solubility (ln $x$) versus reciprocal temperature for $o,p'$-DDE.
TABLE 18.1.1.22.2
Reported octanol-air partition coefficient of \( p,p' \)-DDE at various temperatures

Shoeib & Harner 2002

generator column-GC/MS

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \log K_{OA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10.905</td>
</tr>
<tr>
<td>15</td>
<td>10.361</td>
</tr>
<tr>
<td>20</td>
<td>9.906</td>
</tr>
<tr>
<td>25</td>
<td>9.530</td>
</tr>
<tr>
<td>35</td>
<td>9.196</td>
</tr>
</tbody>
</table>

\( \log K_{OA} = A + B/(T/K) \)

\[ A = -7.492 \]

\[ B = 5116 \]

enthalpy of phase change

\( \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 98.0 \)

FIGURE 18.1.1.22.2 Logarithm of \( K_{OA} \) versus reciprocal temperature for \( p,p' \)-DDE.
Insecticides

18.1.1.23 DDT

Common Name: DDT
Synonym: Agritan, Anofex, Arkotine, Azotox, Bosan supra, Bovidermol, Cesarex, chlorophenoethane, Chlorophenothanum, Chlorophenotoxum, Citox, Clofenotan, Dedelo, Deoval, Deol, Detox, Detoxan, Dibovan, Dichophane, dichlordiphenyltrichloroethane, Didigam, Didimac, Dodat, Dykol, ENT 1506, Estonate, Genitox, Gesafid, Gesapon, Gesarex, Gesarol, Guesarol, Gyron, Havero-extra, Ivoran, Ixodex, Kopsol, Mutoxin, Neocid, Parachlorocidum, PEBI, Pentachlorin, Pentech, p,p'-DDT, 4,4'-DDT, Rukseam, Santobane, Zeidane, Zerdane

Chemical Name: 1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane; 1,1′-(2,2,2-trichloroethylidene)-bis(4-chlorobenzene)

Uses: persistent nonsystemic insecticide with contact and stomach action to control mosquitoes for the eradication of malaria but is now prohibited and displaced with less persistent insecticides on crop application.

CAS Registry No: 50-29-3 (p,p'-DDT, DDT), 789-02-6 (o,p'-DDT)

Molecular Formula: C₁₄H₉Cl₅
Molecular Weight: 354.486

Melting Point (°C):
108.5 (Lide 2003)

Boiling Point (°C):
260 (Lide 2003)

Density (g/cm³ at 20°C):
1.55 (Hadaway et al. 1970; Kenaga 1972)

Molar Volume (cm³/mol):
250 (calculated-density, Chiou 1985)
333.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:

Enthalpy of Fusion, ∆Hₘ (kJ/mol):
27.196 (o,p'-DDT, DSC method, Plato & Glasgow 1969)
26.36 (p,p'-DDT, DSC method, Plato & Glasgow 1969)
26.284 (Ruelle & Kesselring 1997)

Entropy of Fusion, ∆Sₘ (J/mol K):
69.036 (Plato & Glasgow 1969)
70.29 (Hinckley et al. 1990)
72.8 (p,p'-DDT, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:
0.147 (assuming ∆Sₘ = 56 J/mol K., Mackay et al. 1986)
0.130 (20°C, assuming ∆Sₘ = 56 J/mol K, 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):
0.0002–0.001 (15°C, shake flask-bioassay, Richards & Cutkomp 1946)
0.0374 (shake flask-radiometric method, measured range 2–37.5°C, Babers 1955)
≤ 0.0012 (shake flask-radiometric method, Bowman et al. 1960)
0.035 (shake flask-colorimetric, Lipke & Kearns 1960)
0.0012 (Stephen & Stephen 1963)
0.0016 (99% pure DDT isomers plus DDE at rm. temp., shake flask-GC, Robeck et al. 1965)
0.0034 (Biggar et al. 1966)
0.0017 (ultracentrifugation-GC, Biggar et al. 1967)
0.0012–0.0374 (Günther et al. 1968)
0.0017*, 0.006*, 0.025* (shake flask-GC, p,p'-DDT, particle size: 0.01, 0.05, 5.0µ, Biggar & Riggs 1974)
0.004, 0.012, 0.085* (shake flask-GC, o,p'-DDT, particle size: 0.01, 0.05, 5.0µ size or less, Biggar & Riggs 1974)
0.0055 (generator column-GC/ECD, Weil et al. 1974)
0.0017 (Martin & Worthing 1977)
0.0010 (shake flask-GC, Paris et al. 1977)
0.004 (shake flask-nephelometry, Hollifield 1979)
0.0012 (Hartley & Graham-Bryce 1980)
0.040 (shake flask-HPLC, Ellgehausen et al. 1981)
0.0645 (shake flask-GC, Chiou et al. 1982)
0.0023 (generator column-GC, Swann et al. 1983)
0.020 (RP-HPLC-RT correlation, Swann et al. 1983)
0.0031–0.0034 (Verschueren 1983)
0.0055 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
log $[S_i/(mol/L)] = -0.195 - 1454/(T/K)$ (liquid, Passivirta et al. 1999)
0.00023 ± 0.00010  (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
0.0956, 0.149 (o,p'-DDT, supercooled liquid $S_i$: 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):
2.0 × 10−5* (p,p'-DDT, 20°C, effusion manometer, measured range 0–100°C, Balson 1947)
log (P/mmHg) = 14.191 – 6160/(T/K), temp range 66–100°C (Antoine eq., effusion, Balson 1947)
log (P/mmHg) = 13.778 – 6010/(T/K); temp range 50–90°C (Antoine eq., effusion, Dickinson 1947)
0.001973*, 0.002027* (o,p'-DDT, 50.1°C, gas saturation-spec., measured range 50.1–90.2°C, Dickinson 1956)
3.30 × 10−5 (interpolated exptl. data of Balson 1947, Spencer & Cliath 1970; Ballschmiter & Wittlinger 1991)
3.33 × 10−5 (20°C, partition coefficient, Atkins & Eggleton 1971)
2.53 × 10−3 (20°C, Melnikov 1971; Spencer 1973, 1982; Callahan et al. 1979, Mabey et al. 1982)
2.03 × 10−3* (20°C, p,p'-DDT, 30°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1972)
log (P/mmHg) = 14.24 – 6176/(T/K); temp range 20–40°C (p,p'-DDT, 30°C, gas saturation-GC, Antoine eq., Spencer & Cliath 1972; Spencer 1975)
7.37 × 10−4 (o,p'-DDT, 30°C, gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)
2.50 × 10−5 (20°C, Hartley & Graham-Bryce 1980; Worthing & Hance 1991)
5.73 × 10−5 (p,p'-DDT, gas saturation-HPLC/liquid scintillation spectrometry, measured range 20–80°C, Rothman 1980)
2.00 × 10−5 (20–25°C, Weber et al. 1980)
1.50 × 10−4 (20°C, GC, Seiber et al. 1981)
6.0 × 10−4, 1.12 × 10−3 (o,p'-DDT 25, 30°C, capillary GC-RT correlation, Westcott & Bidleman 1981)
4.30 × 10−5 (estimated-relative volatilization rate, Dobbs & Cull 1982)
2.67 × 10−3, 2.67 × 10−5 (20°C, calculated values, Grain 1982)
2.01 × 10−5–2.8 × 10−5 (gas saturation, Jaber et al. 1982)
1.96 × 10−5 (20°C, evaporation rate at 20–60°C, Gückel et al. 1982)
4.31 × 10−5 (20°C, relative loss rate, Dobbs & Cull 1982)
1.61 × 10−3, 1.28 × 10−3 (o,p'-DDT, $P_{gc}$ by GC-RT correlation, different stationary phases, Bidleman 1984)
1.33 × 10−3 (o,p'-DDT, supercooled liquid $P_L$, converted from literature $P_S$ with $\Delta S_{fus}$, Bidleman 1984)
8.30 × 10−4, 4.70 × 10−4 (p,p'-DDT, $P_{gc}$ by GC-RT correlation, different stationary phases, Bidleman 1984)
3.16 × 10−4 (p,p'-DDT, supercooled liquid $P_L$, converted from literature $P_S$ with $\Delta S_{fus}$, Bidleman 1984)
2.48 × 10−5 (20°C, GC-RT correlation, Kim 1985)
1.73 × 10−4 (20°C, supercooled liquid value, Bidleman et al. 1986)
2.50 × 10−5 (Hartley & Kidd 1987; Tomlin 1994)
1.33 × 10−3, 1.83 × 10−3 (o,p'-DDT, supercooled liquid $P_L$, converted from literature $P_S$ with different $\Delta S_{fus}$ values, Hinckley et al. 1990)
Insecticides

1.614 × 10⁻³, 1.035 × 10⁻³ (o,p'‐DDT, P_{GC} by GC‐RT correlation with different reference standards, Hinckley et al. 1990)

\[ \log \left( \frac{P}{P_0} \right) = 12.77 – 4626/(T/K) \] (o,p'‐DDT, supercooled liquid, GC‐RT correlation, Hinckley et al. 1990)

3.16 × 10⁻⁴, 5.12 × 10⁻⁴ (p,p'‐DDT, converted from literature P_{PL} with different D_{fus} values, Hinckley et al. 1990)

8.30 × 10⁻⁴ (p,p'‐DDT, P_{GC} by GC‐RT correlation with eicosane as reference standard, Hinckley et al. 1990)

\[ \log \left( \frac{P}{P_0} \right) = 13.02 – 4865/(T/K) \] (p,p'‐DDT, GC‐RT correlation, supercooled liquid, Hinckley et al. 1990)

6.92 × 10⁻⁴, 2.69 × 10⁻⁴, 9.33 × 10⁻⁴ (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bidleman 1992)

2.27 × 10⁻⁸ (20°C, Montgomery 1993)

3.94 (calculated‐P/C, Mackay & Leinonen 1975)

6.02 (20–25°C, calculated, Thibodeaux 1979)

7.48 (20°C, volatilization rate, Burkhard & Guth 1981)

7.29 (calculated‐P/C, Levins 1981)

5.30 (calculated‐P/C, Mackay & Shiu 1981)

1.60 (calculated‐P/C, Mabey et al. 1982)

3.85 (calculated‐P/C, Thomas 1982)

0.466 (estimated‐group method per Hine & Mookerjee 1975, Tucker et al. 1983)


1.63 (calculated‐P/C, Caron et al. 1984)

1.31 (calculated‐P/C, Mackay et al. 1986)

4.96, 8.18 (calculated‐P/C, Taylor & Glotfelty 1988)

2.36 (20°C, calculated‐P/C, Suntio et al. 1988)

1.28, 1.33 (22–24°C, fog chamber‐conc. ratio‐GC/ECD, Fendinger et al. 1989)

0.862 (23°C, wetted‐wall column‐GC/ECD, Fendinger et al. 1989, 1990)

0.16 (0°C, selected, Cotham & Bidleman 1991)

2.90 (calculated‐P/C, Calamari et al. 1991)

6.0 (calculated‐P/C, Ballschmiter & Wittlinger 1991)

1.55 (calculated‐bond contribution method, Meylan & Howard 1991)

1.31, 0.86 (25°C, 24°C, Iwata et al. 1993)

1.31 (23°C, quoted, Montgomery 1993)

0.843 (p,p'‐DDT, wetted wall column‐GC, Altschuh et al. 1999)

log \left( \frac{H}{(P_{20°C}/m^3/moL)} \right) = 13.02 – 3369/(T/K) (Passivirta et al. 1999)

1.1, 1.1 (p,p'‐DDT, LDV literature‐derived value, FAV final adjusted value, Shen & Wania 2005)

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

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

3.98 (shake flask, Kapoor et al. 1973; Lu & Metcalf 1975)

6.19 (calculated, O’Brien 1975)
<table>
<thead>
<tr>
<th>Value</th>
<th>Method and Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.36</td>
<td>shake flask-GC, Chiou et al. 1982</td>
</tr>
<tr>
<td>4.89</td>
<td>Wolfe et al. 1977; Callahan et al. 1979</td>
</tr>
<tr>
<td>5.98</td>
<td>Kenaga &amp; Goring 1978, 1980; Kenaga 1980b</td>
</tr>
<tr>
<td>6.19</td>
<td>shake flask-GC, Freed et al. 1979</td>
</tr>
<tr>
<td>3.98–6.19</td>
<td>Hansch &amp; Leo 1979</td>
</tr>
<tr>
<td>6.36</td>
<td>shake flask, Karickhoff et al. 1979</td>
</tr>
<tr>
<td>5.75</td>
<td>HPLC-RT correlation, Veith et al. 1979b, 1980; Veith &amp; Kosian 1983</td>
</tr>
<tr>
<td>6.69</td>
<td>Belluck &amp; Felsot 1981</td>
</tr>
<tr>
<td>5.94</td>
<td>shake flask-GC/LC, Ellgehausen et al. 1981</td>
</tr>
<tr>
<td>5.55</td>
<td>HPLC-k correlation, McDuffie 1981</td>
</tr>
<tr>
<td>5.10 ± 0.1</td>
<td>radioactive analysis method, Platford et al. 1982</td>
</tr>
<tr>
<td>5.60</td>
<td>shake flask-GC, Platford 1982, 1983</td>
</tr>
<tr>
<td>5.90</td>
<td>(average of shake flask values, Eadsforth &amp; Moser 1983)</td>
</tr>
<tr>
<td>6.12</td>
<td>(average of HPLC-RT correlation, Eadsforth &amp; Moser 1983)</td>
</tr>
<tr>
<td>6.20</td>
<td>(Elgar 1983)</td>
</tr>
<tr>
<td>5.44</td>
<td>shake flask-GC or LSC, Gerstl &amp; Mingelgrin 1984</td>
</tr>
<tr>
<td>6.40</td>
<td>HPLC-RV correlation, Garst 1984</td>
</tr>
<tr>
<td>5.44</td>
<td>(estimated-HPLC/MS; Burkhard et al. 1985)</td>
</tr>
<tr>
<td>6.22</td>
<td>HPLC-RT correlation, Brooke 1986</td>
</tr>
<tr>
<td>6.06</td>
<td>(RP-HPLC-RT correlation, Chin et al. 1986)</td>
</tr>
<tr>
<td>6.21</td>
<td>HPLC-RT correlation, Eadsforth 1986</td>
</tr>
<tr>
<td>6.19</td>
<td>(RP-HPLC correlation, De Kock &amp; Lord 1987)</td>
</tr>
<tr>
<td>6.51</td>
<td>(HPLC-RT correlation, Liu &amp; Leng 1988)</td>
</tr>
<tr>
<td>6.914 ± 0.030</td>
<td>(p,p'-, shake flask/slow-stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo &amp; Eganhouse 2001)</td>
</tr>
<tr>
<td>6.307 ± 0.045; 6.914 ± 0.030</td>
<td>(shake flask-UV/GC/HPLC, BRE value, RITOX value, inter-laboratory studies, Brooke et al. 1990; received highest ranking from Pontolillo &amp; Eganhouse 2001)</td>
</tr>
<tr>
<td>4.89–6.91</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>5.50</td>
<td>(RP-HPLC correlation, Siebaldi &amp; Finizio 1993)</td>
</tr>
<tr>
<td>6.36</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>8.3064</td>
<td>(o,p'-DDT, calculated-UNIFAC group-interaction, Chen et al. 1993)</td>
</tr>
<tr>
<td>6.91</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>5.65</td>
<td>(o,p'-DDT, RP-HPLC-RT correlation, Finizio et al. 1997)</td>
</tr>
<tr>
<td>5.50</td>
<td>(p,p'-DDT, RP-HPLC-RT correlation, Finizio et al. 1997)</td>
</tr>
<tr>
<td>6.50</td>
<td>(p,p'-DDT, quoted lit., calculated, Passivirta et al. 1999)</td>
</tr>
<tr>
<td>6.65</td>
<td>(mean literature value-basic statistics for uncensored original data, Pontolillo &amp; Eganhouse 2001)</td>
</tr>
<tr>
<td>6.28, 6.39</td>
<td>(p,p'-DDT, LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)</td>
</tr>
</tbody>
</table>

**Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C 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>Method and Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.09, 9.22</td>
<td>(p,p'-DDT, generator column-GC/ECO, calculated-$K_{OW}/K_{AW}$ Harner &amp; Mackay 1995)</td>
</tr>
<tr>
<td>8.70</td>
<td>(calculated-$K_{OW}/K_{AW}$, Wania &amp; Mackay 1996)</td>
</tr>
<tr>
<td>9.93</td>
<td>(p,p'-DDT, calculated, Finizio et al. 1997)</td>
</tr>
</tbody>
</table>

$log K_{OA} = -11.291 + 6266/(T/K)$, temp range 5–35°C (o,p'-DDT, gas saturation-GC, Shoeib & Harner 2002)

<table>
<thead>
<tr>
<th>Value</th>
<th>Method and Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.89*</td>
<td>p,p'-DDT, gas saturation-GC/MS, calculated, measured range 5–45°C, Shoeib &amp; Harner 2002)</td>
</tr>
</tbody>
</table>

$log K_{OA} = -5.63 + 4603/(T/K)$, temp range 5–35°C (p,p'-DDT, gas saturation-GC, Shoeib & Harner 2002)

<table>
<thead>
<tr>
<th>Value</th>
<th>Method and Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.81, 9.73</td>
<td>(p,p'-DDT, LDV literature derived value, FAV final adjusted value, Shen &amp; Wania 2005)</td>
</tr>
</tbody>
</table>

**Bioconcentration Factor, log BCF:**

<table>
<thead>
<tr>
<th>Value</th>
<th>Species and Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.31–6.23</td>
<td>earthworms, Wheatley &amp; Hardman 1968</td>
</tr>
<tr>
<td>2.42</td>
<td>(Cylindrotheca closterium, Keil &amp; Priester 1969)</td>
</tr>
<tr>
<td>4.40; 4.90; 4.40</td>
<td>(Syracostaera carterae; Amphidinium cartaria; Tholassiosira fluviatilis, Cox 1970)</td>
</tr>
<tr>
<td>4.00</td>
<td>(pinfish, Hansen &amp; Wilson 1970)</td>
</tr>
<tr>
<td>4.58</td>
<td>(Atlantic croaker, Hansen &amp; Wilson 1970)</td>
</tr>
</tbody>
</table>
3.94 (soft clam, Butler 1971)
4.20–4.36 (Daphnia magna over concn. gradient 8 µg/L to 1.1 mg/L, Crosby & Tucker 1971)
5.00 (Daphnia magna at water level 80 ng/L, Johnson et al. 1971)
4.27 (Daphnia magna, wet wt. basis, Crosby & Tucker 1971)
4.45 (Daphnia magna, wet wt. basis, Johnson et al. 1971)
4.08–4.60 (fishes, Menzie 1972)
4.93, 4.54 (Gambusia, Physa, Metcalf et al. 1973)
4.68 (oyster, Parrish 1974)
4.79 (Ankistrodesmus, Neudorf & Khan 1975)
3.52–3.63, 3.11–3.43 (bacteria, algae, Wolfe et al. 1977)
3.14 (trout muscle, Branson 1978)
4.47 (fathead minnow, 32-d exposure, Veith et al. 1979b, 1980)
4.72 (bluegill sunfish-kinetic value, Bishop & Maki 1980)
4.79, 4.93 (fish: flowing water, static water; Kenaga 1980a,b; Kenaga & Goring 1980)
4.35; 4.43 (calculated-S, calculated-K OC, Kenaga 1980a)
–0.045 (average beef fat diet, Kenaga 1980b)
4.15 (pulex, Kenaga & Goring 1980)
4.11 (algae, estimated, Baughman & Paris 1981)
2.95–3.03; 3.02–3.13 (Rhodotorulus solani, Alfafa tissue, Baughman & Paris 1981)
2.10 (Triaenodes tardus, Belluck & Felsot 1981)
5.38 (calculated-K OW, Briggs 1981)
5.11 (selected, Schnoor & McAvoy 1981, Schnoor 1992)
4.36, 4.15, 4.43 (estimated-S, calculated-K OW, calculated-K OC, Bysshe 1982)
4.47, 4.43 (fish: quoted, correlated, Mackay 1982)
4.37 (mussels, quoted average, Geyer et al. 1982)
6.90 (microorganism-water, Mabey et al. 1982)
2.30, 4.08 (trout, pinfish, Verschueren 1983)
4.71 (15°C, rainbow trout, Davies & Dobbs 1984)
5.00 (25°C, fathead minnow-steady state, Davies & Dobbs 1984)
4.15 (activated sludge, Freitag et al. 1984)
3.97, 3.46, 4.15 (algae, fish, activated sludge, Klein et al. 1984)
3.97, 3.28, 4.15 (algae, golden ide, activated sludge, Freitag et al. 1985)
4.97 (Oncorhynchus mykiss, Muir et al. 1985)
3.91, 3.08 (rainbow trout: kinetic, steady-state, Oliver & Niimi 1985)
4.47, 4.56 (oyster, calculated-K OW & models, Zaroojian et al. 1985)
3.24–5.00 (p,p′-DDT, benthic macroinvertebrates, Reich et al. 1986)
3.44–5.71 (o,p′-DDT, benthic macroinvertebrates, Reich et al. 1986)
4.08 (Selenastrum capricornutum, Mailhot 1987)
6.50 (zooplankton, chum salmon; Kawano et al. 1988)
–1.55 (beef biotransfer factor log B b, correlated-K OW from Radeleff et al. 1952 & Kenaga 1980, Travis & Arms 1988)
–1.80 (vegetation, correlated-K OW from Beall & Nash 1972 & Voerman & Besemer 1975, Travis & Arms 1988)
5.28, 7.64 (dry leaf, wet leaf, Bacci et al. 1990)
4.47, 4.30 (quoted, calculated, Banerjee & Baughman 1991)
4.72 (selected, Chessells et al. 1992)
–0.155, –1.0 (earthworms, quoted, field/lab., Menzie et al. 1992)
–1.0, –0.602 (earthworms, field leaf litter, calculated-model, Menzie et al. 1992)
4.81, 4.86, 4.95, 4.99 (Oncorhynchus mykiss, Muir et al. 1994)
4.05, 2.85, 3.70 (algae Selenastrum capricornutum, water flea Daphnia magna, catfish Ictalurus melas, wet wt. basis, Wang et al. 1996)
3.97, 4.81 (algae Chlorella: wet wt basis, dry wt basis, p,p′-DDT, Geyer et al. 2000)
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4.45, 6.45 (Daphnia: wet wt basis, lipid wt basis, p,p′-DDT, Geyer et al. 2000)
5.14, 7.06 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, p,p′-DDT, Geyer et al. 2000)
4.97, 6.67 (rainbow trout: wet wt basis, lipid wt basis, p,p′-DDT, Geyer et al. 2000)
>4.57, >5.55 (fathead minnow, 10.5% lipid, 28-d: wet wt basis, lipid wt basis, o,p′-DDT, Geyer et al. 2000)

Bioaccumulation Factor BAF:
1.27 (bioaccumulation factor log BAF, adipose tissue in male Albino rats, Berdanier & de Dennis 1977)
4.20; 3.539; 3.35 (log BF-bioaccumulation factor of algae; catfish; daphnids, Ellgehausen et al. 1980)
5.10 (fish, reported as log BAF,w, LeBlanc 1995)

Sorption Partition Coefficient, log K_OC:
3.93 (sediment, Wolfe et al. 1977)
5.38 (calculated-K_{OC}, Kenaga 1980)
5.16 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
5.38 (Kenaga & Goring 1980; quoted, Hodson & Williams 1988)
5.18 (average 3 soils, HPLC-RT correlation, McCall et al. 1980)
5.39 (average soils/sediments, Rao & Davidson 1980)
5.20, 5.18, 5.18; 5.18 (commerce soil, Tracy soil, Catlin soil; average soil, McCall et al. 1980)
5.00 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
5.62; 6.81, 5.80 (estimated-S; estimated-S and mp, calculated-K_{OC}, Karickhoff 1981)
6.59 (calculated-K_{OC}, Mabey et al. 1982)
5.38 (soil, Thomas 1982; quoted, Nash 1988)
5.20 (Pavlou & Weston 1983, 1984)
5.18, 4.64 (soil slurry method, HPLC-RT correlation, Swann et al. 1983)
5.38 (soil, Jury et al. 1984; quoted, Mackay & Stiver 1991)
5.38, 5.33 (soil: quoted, calculated-MCI χ, Sabljic 1984)
5.61 (Caron et al. 1984)
5.39 (soil, estimated, Karickhoff 1985)
6.00 (best estimate at low sediment concn., Karickhoff 1985)
5.11–5.45 (Aldrich humic acid, Landrum et al. 1984)
4.28–4.66 (natural water, Landrum et al. 1984)
5.61 ± 0.11 (Chiou et al. 1987; quoted, Chin et al. 1991)
6.03 (predicted-K_{OC}, Chiou et al. 1987)
5.39 (selected, Elzerman & Coates 1987)
3.94 (calculated-MCI χ, Gerstl & Helling 1987)
5.38 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
5.38, 5.34 (quoted, calculated- MCI χ, Bahnick &Doucette 1988)
5.63 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
4.09 (calculated-K_{OC} as per Kenaga & Goring 1980, Chapman 1989)
5.15–6.26 (Montgomery 1993)
6.59 (estimated-QSAR and SPARC, Kollig 1993)
5.31 (soil, calculated-MCI χ, Sabljic et al. 1995)
5.63; 5.34 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
5.17 (p,p′-DDT, soil, estimated-general model, Gramatica et al. 2000)
6.08 (p,p′-DDT, average values for sediments OC ≥ 0.5%, Delle Site 2001)
5.63, 5.54 (p,p′-DDT, soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
5.20 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Sorption Partition Coefficient, log K_{OM}:
5.14 (exptl., Briggs 1981)
4.24 (calculated-Parachor, Briggs 1981)
4.88 – 5.41 (Mingelgrin & Gerstl 1983)
5.69, 5.59, 5.69 (average soil, sediment, soil and sediment, Gerstl & Mingelgrin 1984)
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 3.7$ d for water depth of 1 m (Mackay & Wolkoff 1973);

initial rate constant $k = 6.9 \times 10^{-4}$ h$^{-1}$ and predicted rate constant $k = 1.2 \times 10^{-3}$ h$^{-1}$ from soil with $t_{1/2} = 578$ h;

half-flux values times, 0.3 d from field study, 0.3–12 d from microagroecosystem, >80–1000 d from laboratory data (Nash 1983).

Photolysis: midsummer direct photolysis $k = 8.5 \times 10^{-8}$ s$^{-1}$ with $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{1/2} > 150$ yr (12-h days) in water in the Central U.S. (Zepp et al. 1976) using fungus and either 254 or 300 nm UV light, more than 97% initial added amounts were metabolized in 3 wk of incubation (Katayama & Matsumura 1991).

Oxidation: $t_{1/2} = 22$ yr, estimated first-order half-life in aquatic environment (Callahan et al. 1979)

$< 3600$ M$^{-1}$ h$^{-1}$ for singlet oxygen, $k = 3600$ M$^{-1}$ h$^{-1}$ for RO$_2$ (Mabey et al., 1982)

photooxidation $t_{1/2} = 17.7$–177 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

photooxidation $t_{1/2} = 168$–8400 h in water, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Howard et al. 1991)

Hydrolysis: $k_{\text{alkaline}} = 9.90 \times 10^{-3}$ M$^{-1}$ s$^{-1}$ at 27°C corresponds to $t_{1/2} = 81$ d at pH 9, $k_{\text{neutral}} = 1.9 \times 10^{-9}$ s$^{-1}$ corresponds to $t_{1/2} = 12$ yr in 5% acetonitrile-water at pH 5 and 27°C (Wolfe et al. 1977b)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 2$–15.6 yr based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)

$\Sigma$DDT in the Great Lake’s atmosphere. $t_{1/2} = 17.0 \pm 6.8$ yr at Eagle Harbor, $t_{1/2} = 8.2 \pm 1.4$ yr at Sleeping Bear Dunes and $t_{1/2} = 7.1 \pm 1.0$ yr at Sturgeon Point (Buehler et al. 2004).

Surface water: dehydrochlorination rate constant $k = 1.75 \times 10^{-2}$ h$^{-1}$ for 1 ppm $p,p'$-DDT and $k = 1.65 \times 10^{-2}$ h$^{-1}$ for 1 ppm $o,o'$-DDT both at 21 ± 2°C and pH 12.8, in 0.1 N NaOH solution (Choi & Chen 1976);

degradation $t_{1/2} = 8$ yr in water at 27°C (Wolfe et al. 1977);

midsummer direct photolysis $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{1/2} > 150$ yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)
$t_1/2 = 73.9$ h for a pond 1 m deep (Branson 1978);
$t_1/2 = 168–8400$ h, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Callahan et al. 1979; quoted, Howard et al. 1991; Mortimer & Connell 1995);
estimated $t_1/2 = 110$ and 56 d for o.p- and p,p-DDT, respectively, in surface waters in case of first order reduction process may be assumed in the Netherlands (Zoeteman et al. 1980)
degradation $t_1/2 \sim 10$ yr average from the loss rates in Lake Michigan (Bierman & Swain 1982).

Ground water: $t_1/2 = 16$ d to 31.3 yr, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).

Sediment: $t_1/2 = 3$ to 5 yr (Bierman & Swain 1982); $t_1/2 = 21$ yr (conversion of $p,p'$/DDT to $p,p'-DDE$ in sediment, Oliver et al. 1989); $t_1/2 = 78800$ h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).

Soil: $t_1/2 = 2–15.6$ yr, based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991);
average $t_1/2 \sim 12$ yr in 3 different soils for $\sim 50$ ppm in soil (Nash & Woolson 1967);
estimated persistence of 4 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
field $t_1/2 = 173$ d when incorporated into soil (Willis et al. 1971; quoted, Nash 1983);

microagroecosystem $t_1/2 > 50$ d with open cotton canopy (quoted, Nash 1983);
persistence of more than 36 months (Wauchope 1978);
$t_1/2 > 50$ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
estimated first-order $t_1/2 = 14.6$ yr from biodegradation rate constant $k = 0.00013$ d$^{-1}$ from soil incubation studies and $t_1/2 = 198$ d from rate constant $k = 0.0035$ d$^{-1}$ from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);
very persistent in soils with $t_1/2 > 100$ d (Willis & McDowell 1982);

microagroecosystem $t_1/2 > 50$ d in moist fallow soil (Nash 1983);
$t_1/2 = 3837$ d from screening model calculations (Jury et al. 1984, 1987a, b; Jury & Ghorati 1989);
$t_1/2 = 173$ d from field study, $t_1/2 > 50$ d from microagroecosystem, $t_1/2 = 116$ d from laboratory data (Nash 1985);
$t_1/2 = 3800$ d (Jury et al. 1987; quoted, Montgomery 1993);
reaction $t_1/2 = 3837$ d and overall $t_1/2 = 9.4$ yr (Mackay & Stiver 1991);
estimated field $t_1/2 = 2000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_1/2 = 14.0$ and 12.0 yr for control and sludge-amended Luddington soils, respectively, for $o,p'$-DDT, and $t_1/2 = 11.8$ and 10.5 yr for control and sludge-amended Luddington soils, respectively, for $p,p'$-DDT (Meijer et al. 2001).

Biota: field $t_1/2 = 15$ d in fruit leaves (Decker et al. 1950; quoted, Nash 1983);

microagroecosystem $t_1/2 = 29$ d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
$t_1/2 = 915$ h from fish compared with calculated value of $t_1/2 = 517$ h from regression (Neely 1980);
$t_1/2 = 0.70$ h in algae, $t_1/2 = 3.65$ d in catfish and $t_1/2 = 315$ h in daphnids (Ellgehausen et al. 1980);
$t_1/2 = 340$ d in rainbow trout (Oliver & Niimi 1985);

biochemical $t_1/2 = 3837$ d (Jury et al. 1987a, b; Jury & Ghodrati 1989);

biological $t_1/2 = 77$ d for trout, $t_1/2 = 31$ d for salmon, $t_1/2 = 4$ d for catfish (Niimi 1987).
### TABLE 18.1.1.23.1
Reported aqueous solubilities of DDT at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>p,p'-DDT</th>
<th>o,p'-DDT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S/g·m–3</td>
<td>S/g·m–3</td>
</tr>
<tr>
<td>0.01µm</td>
<td>0.001</td>
<td>0.0025</td>
</tr>
<tr>
<td>0.05µm</td>
<td>0.0017</td>
<td>0.006</td>
</tr>
<tr>
<td>5.0µm</td>
<td>0.0026</td>
<td>0.013</td>
</tr>
<tr>
<td></td>
<td>0.0039</td>
<td>0.0275</td>
</tr>
</tbody>
</table>

**FIGURE 18.1.1.23.1A** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for p,p'-DDT.

**FIGURE 18.1.1.23.1B** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for o,p'-DDT.
### Table 18.1.1.23.2
Reported vapor pressures of DDT at various temperatures and the coefficients for the vapor pressure equations

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

1. Balson 1947  
   effusion manometer  
   \[
   \begin{array}{c|c|c}
   t/°C & P/Pa & p,p'-DDT \\
   \hline
   0 & 5.87 \times 10^{-7} & 71.0 \\
   10 & 3.60 \times 10^{-6} & 71.0 \\
   20 & 2.00 \times 10^{-5} & 71.0 \\
   30 & 9.60 \times 10^{-4} & 70.7 \\
   40 & 4.27 \times 10^{-3} & 70.7 \\
   50 & 1.77 \times 10^{-2} & 70.7 \\
   60 & 4.00 \times 10^{-1} & 71.3 \\
   70 & 0.0231 & 71.3 \\
   80 & 0.0301 & 50.1 \\
   90 & 0.224 & 50.1 \\
   100 & 0.640 & 60.1 \\
   \end{array}
   \]

   Dickinson 1956  
   gas saturation-spec.  
   \[
   \begin{array}{c|c|c}
   t/°C & P/Pa & p,p'-DDT \\
   \hline
   20 & 2.03 \times 10^{-5} & 71.0 \\
   30 & 9.68 \times 10^{-5} & 71.0 \\
   40 & 4.43 \times 10^{-4} & 71.0 \\
   50 & 2.0 \times 10^{-3} & 71.0 \\
   60 & 6.40 \times 10^{-3} & 71.0 \\
   80 & 0.060 & 80.1 \\
   \end{array}
   \]

   Spencer & Cliath 1972  
   gas saturation-GC  
   \[
   \begin{array}{c|c|c}
   t/°C & P/Pa & p,p'-DDT \\
   \hline
   20 & 2.03 \times 10^{-5} & 71.0 \\
   30 & 9.68 \times 10^{-5} & 71.0 \\
   40 & 4.43 \times 10^{-4} & 71.0 \\
   50 & 2.0 \times 10^{-3} & 71.0 \\
   60 & 6.40 \times 10^{-3} & 71.0 \\
   80 & 0.060 & 80.1 \\
   \end{array}
   \]

   Rothman 1980  
   radiotracer transpiration  
   \[
   \begin{array}{c|c|c}
   A & 14.24 & 80.1 \\
   B & 6176 & 80.1 \\
   \end{array}
   \]

2.  
   \[
   \Delta H_{\text{sub}} = 100.6 \text{ kJ/mol}
   \]

3.  
   \[
   \begin{array}{c|c}
   \text{eq. 1 P/mmHg} & 80.4 \\
   A & 14.191 \\
   B & 6160 \\
   \end{array}
   \]

4.  
   \[
   \begin{array}{c|c}
   \text{temp range: 66–100°C} & 80.4 \\
   88.8 & 0.07599 \\
   88.8 & 0.2039 \\
   90.2 & 0.1933 \\
   90.2 & 0.2200 \\
   90.2 & 0.2346 \\
   \end{array}
   \]
TABLE 18.1.1.23.2 (Continued)

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>gas saturation-GC</td>
<td>capillary GC-RT correlation</td>
<td>gas saturation-GC/ECD</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>o,p′-DDT</td>
<td>30</td>
<td>1.17 × 10⁻³</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1.12 × 10⁻³</td>
</tr>
<tr>
<td>p,p′-DDT</td>
<td>30</td>
<td>1.87 × 10⁻¹</td>
</tr>
</tbody>
</table>

enthalpy of sublimation:
\[ \Delta H_{\text{sub}} = 120.2 \text{ kJ/mol} \]

FIGURE 18.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for p,p′-DDT.
### TABLE 18.1.1.23.3
Reported octanol-air partition coefficients of DDT at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>p,p’-DDT</th>
<th>o,p’-DDT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-GC/MS</td>
<td>generator column-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>log $K_{OA}$</td>
<td>t/°C</td>
</tr>
<tr>
<td>15</td>
<td>10.09</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>9.879</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>35</td>
</tr>
</tbody>
</table>

\[ \log K_{OA} = A + B/(T/K) \]

- A: -3.20
- B: 3954

\[ \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 75.7 \]

\[ \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 88.1 \]

\[ \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 87.9 \]

**FIGURE 18.1.1.23.3A** Logarithm of $K_{OA}$ versus reciprocal temperature for p,p'-DDT.
FIGURE 18.1.23.3B Logarithm of $K_{OA}$ versus reciprocal temperature for $o,p'$-DDT.
18.1.1.24 Deltamethrin

Common Name: Deltamethrin
Synonym: Decis, K-Othrin, Butoss, RU 22074, Cislin, Crackdown
Chemical Name: \( S-\alpha\text{-cyano-3-phenoxybenzyl (1R,3R)}\text{-3-(2,2-dibromovinyl)-2,2-dimethyl cyclopropan-1-carboxylate} \)
CAS Registry No: 52918-63-5
Uses: insecticide (pyrethroid)
Molecular Formula: C\(_{22}\)H\(_{19}\)Br\(_2\)NO\(_3\)
Molecular Weight: 505.199
Melting Point (°C):
- 98–101 (Hartley & Kidd 1987)
- 98–102 (Tomlin 1994)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
- 0.55 (25°C, bulk density, Tomlin 1994)
Molar Volume (cm\(^3\)/mol):
Dissociation Constant, pK\(_a\):
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):
- <0.002 (20°C, Hartley & Kidd 1987)
- <0.0002 (Tomlin 1994)
Vapor Pressure (Pa at 25°C):
- 2.0 × 10\(^{-6}\) (Hartley & Kidd 1987)
- <1.33 × 10\(^{-5}\) (Tomlin 1994)
Henry’s Law Constant (Pa·m\(^3\)/mol):
- 12.6 (gas stripping-LSC, Muir et al. 1985a)
Octanol/Water Partition Coefficient, log K\(_{\text{OW}}\):
- 5.20 (HPLC-RT correlation, Muir et al. 1985b)
- 6.20 (shake flask, Log P Database, Hansch & Leo 1987)
- 6.21 (HPLC-RT correlation, Hu & Leng 1992)
- 6.20 (recommended, Sangster 1993)
- 4.60 (Tomlin 1994)
- 6.20 (recommended, Hansch et al. 1995)
- 5.74 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
Octanol/Air Partition Coefficient, log K\(_{\text{OA}}\):
Bioconcentration Factor, log BCF or log K\(_b\):
- 1.53–3.0 (fathead minnows, Muir et al. 1985a)
- 2.06–2.48 (chironomid larvae, Muir et al. 1985b)
- 2.62, 2.70 (\textit{Oncorhynchus mykiss}, flow-through condition, quoted, Devillers et al. 1996)
Insecticides

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

3.66–4.21 \hspace{1em} (Tomlin 1994)

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

Volatilization:

Photolysis: \( t_{\scriptstyle 1/2} = 9 \) d in soil (Tomlin 1994).

Oxidation:

Hydrolysis: more stable in acidic than in alkaline media with \( t_{\scriptstyle 1/2} = 2.5 \) d at pH 9 and 25°C (Tomlin 1994).

Biodegradation: microbial degradation half-life are, \( t_{\scriptstyle 1/2, \text{(aerobic)}} = 21–25 \) d, \( t_{\scriptstyle 1/2, \text{(anaerobic)}} = 31–36 \) d in laboratory; \( t_{\scriptstyle 1/2} < 23 \) d in field (Tomlin 1994)

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: \( t_{\scriptstyle 1/2} = 2–4 \) d in water of small outdoor ponds (Muir et al. 1985);

more stable in acidic than in alkaline media with \( t_{\scriptstyle 1/2} = 2.5 \) d at pH 9 and 25°C (Tomlin 1994).

Ground water:

Sediment:

Soil: undergoes microbial degradation within 1–2 wk (Hartley & Kidd 1987)

microbial degradation half-life are, \( t_{\scriptstyle 1/2, \text{(aerobic)}} = 21–25 \) d, \( t_{\scriptstyle 1/2, \text{(anaerobic)}} = 31–36 \) d in laboratory; \( t_{\scriptstyle 1/2} < 23 \) d in field; photolysis \( t_{\scriptstyle 1/2} = 9 \) d (Tomlin 1994).

Biota:
18.1.1.25 Demeton

Common Name: Demeton
Synonym: Bayer 8169, Demeton-O, E-1059, mercaptophos, Systox-O
Chemical Name: \(O,O\)-diethyl-\(O\)-(2-ethylthioethyl)phosphorothioate mixture with \(O,O\)-diethyl-S-(2-ethylthioethyl)-phosphorothioate
Uses: insecticide to control sucking insects and mites in a wide range of crops, including fruit, nuts, vegetables, ornamentals, and field crops; also used as acaricide.
CAS Registry No: 8065-48-3, 298-03-3 demeton-O, systox-O
126-75-0 demeton-S, systox-S
Molecular Formula: \(\text{C}_8\text{H}_{19}\text{O}_3\text{PS}_2\)
Molecular Weight: 258.339
Melting Point (°C): pale yellow oil (Hartley & Kidd 1987)
Boiling Point (°C):
- 123 (Khan 1980)
- 92–93 (at 0.15 mmHg, Hartley & Kidd 1987)
Density (g/cm\(^3\) at 20°C):
- 1.119 (25°C, Spencer 1982)
- 1.119–1.132 (Hartley & Kidd 1987)
Molar Volume (cm\(^3\)/mol):
- 264.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK\(_a\):
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/m\(^3\) or mg/L at 25°C or as indicated):
- 60 (20°C, Kenaga 1980a)
- 60 (22°C, Khan 1980; Worthing & Walker 1983)
- 100 (20–25°C, Willis & McDowell 1982)
- 60 (rm. temp., Spencer 1982; Hartley & Kidd 1987)
Vapor Pressure (Pa at 25°C or as indicated):
- 0.0973, 0.0987 (30°C, demeton-O, demeton-S, Eichler 1965)
- 0.00331, 0.0347 (20°C, demeton-O, demeton-S, Melnikov 1971)
- 0.00373, 0.0347 (20°C, demeton-O, demeton-S, Hartley & Graham-Bryce 1980)
- 0.0331 (Khan 1980)
- 0.033 (20°C, Spencer 1982)
- 0.0167, 0.00707 (20°C, demeton-O, demeton-S, GC-RT correlation, Kim 1985)
- 0.034 (20°C, Hartley & Kidd 1987)
- 0.030 (20°C, selected, Suntio et al. 1988)
- 0.1333 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
- 0.130 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):
Octanol/Air Partition Coefficient, \(\log K_{\text{oa}}\):
Bioconcentration Factor, log BCF:
1.79  
(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.66  
(soil, calculated-S, Kenaga 1980)
1.85  

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Oxidation: calculated rate constant \( k = 128 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Half-Lives in the Environment:
Soil: selected field t_{1/2} = 15 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
18.1.1.26 Dialifor

Common Name: Dialifor
Synonym: dialiphos, Torak
Chemical Name: \( S-(2\text{-chloro-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl}) \ O,\text{O-diethyl phosphorodithioate} \)
CAS Registry No: 10311-84-9
Uses: insecticide/acaricide
Molecular Formula: \( \text{C}_{14}\text{H}_{17}\text{ClNO}_{4}\text{PS}_{2} \)
Molecular Weight: 393.846
Melting Point (°C):
68 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\)) at 20°C:
Molar Volume (cm\(^3\)/mol):
Dissociation Constant, \( pK_a \):
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: 0.379 (mp at 68°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C):
0.18 (Chiou et al. 1977; Kenaga 1980b)
< 1.0 (Hartley & Kidd 1987)
0.18 (room temp., Montgomery 1993)
Vapor Pressure (Pa at 25°C):
0.133 (35°C, Hartley & Kidd 1987)
1.08 \times 10^{-7} (20°C, Montgomery 1993)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
0.142 (20°C, calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
4.69 (shake flask-GC, Chiou et al. 1977; quoted, Rao & Davidson 1980; Sangster 1993)
4.69 (Montgomery 1993)
Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):
Bioconcentration Factor, log \( BCF \) or log \( K_B \):
3.21 (calculated, Kenaga 1980b)
Sorption Partition Coefficient, log \( K_{\text{oc}} \):
4.04 (soil, calculated, Kenaga 1980b)
4.05 (Montgomery 1993)
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{\text{1/2}} \):
Hydrolysis: \( t_{\text{1/2}} = 14 \text{ h at 20°C and pH 7.4, } t_{\text{1/2}} = 1.8 \text{ h at 37.5°C and pH 7.4 (Montgomery 1993).} \)
Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{1/2} = 14$ h at 20°C and pH 7.4, $t_{1/2} = 1.8$ h at 37.5°C and pH 7.4 (Montgomery 1993).
Ground water:
Sediment:
Soil:
Biota: rapidly eliminated in animal (Hartley & Kidd 1987).
18.1.1.27 Diazinon

Common Name: Diazinon
Synonym: Alfa-Tox, AG-500, Basudin, Bazinon, Bazuden, Ciazinon, Dacutox, Dassitox, Dazzel, Desapon, Dianon, Diater, Diaterr-fos, Diazitol, Diazide, Diazol, Dicid, Dimpylate, Dipofene, Dizinon, Dyzol, ENT 19507, Flytrol, G 301, Gardentox, Geigy 24480, Kayazinon, Kayazol, NA 2763, Nedicisol, Neocidol, Nipsan, Nucidol, Sarolex, Spectracide

Chemical Name: \( O,O\text{-diethyl } O\text{-2-isopropyl-6-methylpyrimidin-4-yl phosphorothioate; } O,O\text{-diethyl-}\) \(O\text{-}2\text{-isopropyl-6-methyl 4-pyrimidinyl) phosphorothioate; } O,O\text{-diethyl 2-isopropyl-4-methylpyrimidinyl-6-thiophosphate}\)

Uses: nonsystemic insecticide to control flies, aphids and spider mites in soil, fruit, vegetables and ornamentals; also used as acaricide.

CAS Registry No: 333-41-5
Molecular Formula: \( C_{12}H_{21}N_{2}O_{3}PS \)
Molecular Weight: 304.345
Melting Point (°C):
- colorless oil (Hartley & Kidd 1987; Tomlin 1994)

Boiling Point (°C):
- 125 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
- 83–84 (at 0.0002 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm³ at 20°C):
- 1.11 (Worthing & Hance 1991)
- 1.116–1.118 (Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):
- 320.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, \( pK_a \):
- < 2.5 (Albert 1963; Perrin 1989; Somasundaram et al. 1991; Montgomery 1993)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
- 87.5 (Rordorf 1989)

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), \( F \): 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 68.8 (22°C, shake flask-GC, Bowman & Sans 1979, 1983a, b)
- 40 (Hartley & Graham-Bryce 1980)
- 40 (22°C, Khan 1980)
- 40 (20°C, Windholz 1983)
- 53.5, 43.7 (20°C, 30°C, Montgomery 1993)
- 52.36, 103.8 (supercooled liquid \( S_L \); literature-derived value LDV, final adjusted value FAV, Muir 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):
- 0.0187 (Margot & Stammbach 1964)
- 0.0111 (20°C, Wolfdietrich 1965)
- 0.0112 (20°C, Melnikov 1971)
Insecticides

0.0161  (gas saturation, Heiber & Szelagiewicz 1976)
0.020  (gas saturation method, measured range 32–73°C, Marti 1976)
\log (P/mmHg) = 11.46 – 4569.55/(T/K), temp range 32–73°C (Marti 1976)
0.0187  (Worthing 1979)
0.019  (20°C, Hartley & Graham-Bryce 1980)
0.0187  (Khan 1980)
0.00971  (20°C, volatilization rate, Burkhard & Guth 1981)
0.00236–0.00469  (20°C, GC, Seiber et al. 1981)
0.0109*  (gas saturation-GC, measured range 25.3–45.0°C, Kim et al. 1984)
\log (P/mmHg) = 9.3871 – 4014.67/(T/K); temp range 25.3–45°C (gas saturation, Kim et al. 1984)
0.0064  (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temp, Kim et al. 1984)
0.0024  (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
9.7 × 10^{-5}  (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
0.014*  (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
\log (P/Pa) = 13.482 – 4571.2/(T/K); measured range 32.4–140°C (liquid, gas saturation-GC, Rordorf 1989)
0.020  (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
0.008  (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0113  (20°C, Montgomery 1993)
0.012  (20°C, Tomlin 1994)
0.0123  (liquid P_L, GC-RT correlation, Donovan 1996)
0.011  (gradient GC method; Tsuzuki 2000)
0.011; 0.0339, 0.0513  (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)
0.014, 0.0073  (supercooled liquid P_L; literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
0.074  (20°C, volatilization rate, Burkhard & Guth 1981)
0.0114  (calculated, Adachi et al. 1984)
0.124  (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.0114  (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)
0.0669  (20°C, calculated-P/C, Suntio et al. 1988)
0.1438  (calculated-P/C, Taylor & Glotfelty 1988)
0.0138, 0.0101  (22–24°C, fog chamber-GC/ECD: drain water, cyclone water, Fendinger et al. 1989)
0.007  (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
0.0114  (20°C, calculated-P/C, Montgomery 1993)
0.0406  (calculated-P/C, this work)
0.0338*  (20°C, gas stripping-GC/MS, measured range 283–301 K, Feigenbrugel et al. 2004)
\frac{H/(M atm^{-1})}{(7.2 ± 0.5) × 10^{-15}} \exp[(11900 ± 700)/(T/K)]; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)
0.0108, 0.0216  (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
3.02  (Rao & Davidson 1980)
3.11  (shake flask-UV, Lord et al. 1980)
3.11  (20°C, shake flask-UV, Briggs 1981)
3.81  (shake flask-GC, Bowman & Sans 1983b)
1.92  (Veith & Kosian 1983)
3.02  (shake flask, Log P Database, Hansch & Leo 1987)
3.02–3.81  (Montgomery 1993)
3.70  (RP-HPLC-RT correlation, Saito et al. 1993)
3.58  (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.30  (Tomlin 1994)
Octanol/Air Partition Coefficient, $\log K_{oa}$:
- 3.81 (recommended, Hansch et al. 1995)
- 4.23 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 3.81 (literature-derived value LDV, Muir et al. 2004)

Bioconcentration Factor, $\log BCF$:
- 2.39 (motsugo, Kanazawa 1975)
- 1.54 (fish in flowing water, Alison & Hermanutz 1977)
- 2.18, 1.56 (topmouth gudgeon, silver crucian carp, Kanazawa 1978, 1981)
- 1.81; 1.24 (carp; guppy, Kanazawa 1978)
- 0.69, 1.23, 0.77 (crayfish, red snail, pond snail, Kanazawa 1978)
- 1.83; 0.954 (fish; invertebrates, Kanazawa 1978)
- 1.89 (calculated-S, Kenaga 1980)
- 2.75 (earthworms, Lord et al. 1980)
- 2.08, 1.80 (carp, rainbow trout, Seguchi & Asaka 1981)
- 1.41, 0.477 (loach, shrimp, Seguchi & Asaka 1981)
- 1.81; 1.24; 2.18 (carp; guppy; topmouth gudgeon, Veith & Kosian 1983)
- 2.32 (topmouth gudgeon, Kanazawa 1983)
- 2.30 (sheepshead minnow, Zaroogian et al. 1985)
- 1.46 (Isnard & Lambert 1988)
- 0.59 (vegetation, correlated-$K_{ow}$, Nash 1974)
- 2.39 (willow shiner, Tsuda et al. 1989; Tsuda et al. 1992)
- 1.81, 2.08 (carp, De Bruijn & Hermens 1991)
- 1.38, 1.81, 1.81 (loach, motsugo, rainbow trout, De Bruijn & Hermens 1991)
- 2.16–2.33 (sheepshead minnow, De Bruijn & Hermens 1991)
- 1.56, 2.18 (silver crucian carp, topmouth gudgeon, De Bruijn & Hermens 1991)
- 2.18, 1.79 (pale chub, ayu sweetfish, calculated-field data, Tsuda et al. 1992)
- 3.20 (eel, Sancho et al. 1993)
- 2.02 (killifish $Oryzias latipes$, after 24–72 h exposure, Tsuda et al. 1995)
- 1.34, 1.45 ($Oryzias latipes$, Tsuda et al. 1995; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:
- 2.76 (calculated-S as per Kenaga & Goring 1978, Kenaga)
- 2.93 (Rao & Davidson 1980)
- 2.28, 2.40 (average of 3 soils, 1 sediment, Sharom et al. 1980)
- 2.36 (soil, sorption isotherm, converted from reported $\log K_{OM}$ of 2.12, Briggs 1981)
- 2.36 (estimated, Lyman et al. 1982; quoted, Howard 1991; Lohninger 1994)
- 2.93 (screening model calculations, Jury et al. 1987b; Jury & Ghodrati 1989)
- 2.40 (average of 2 soils, Kanazawa 1989)
- 2.12, 3.27 (reported, estimated as $\log K_{OM}$, Magee 1991)
- 2.75, 3.13 (soil, quoted exptl., calculated-$\chi$ and fragment contribution, Meylan et al. 1992)
- 2.76 (soil, average value, Dowd et al. 1993)
- 3.00–3.27 (Montgomery 1993)
- 2.75 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.75, 3.05 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.74, 2.64, 2.90 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)
- 3.12–3.16 (sediments from San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization: mostly dissipated through volatilization with $t_{1/2} = 19$ d from soil (Glotfelty et al. 1990).
Photolysis: calculated $t_{1/2} = 15$ d for photolysis in an aqueous buffer solution at pH 7 and 25°C under UV light for 24 h (Burkhard & Guth 1979; quoted, Montgomery 1993);

$t_{1/2} = 41$ d without addition of humic substances; $t_{1/2} = 9$ d and $t_{1/2} = 5$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994)

Photodegradation ($\lambda > 290$ nm) half-lives in various diazinon aqueous solutions: $t_{1/2} \sim 1$ d river water exposed to sunlight, $t_{1/2} \sim 5$ d lake water exposed to sunlight and $t_{1/2} \sim 5.5$ d with humic acid exposed to sunlight (Mansour et al. 1997)

Photolytic $k = 2.39 \times 10^{-3}$ h$^{-1}$ with $t_{1/2} = 290$ h in moist sandy soil, $k = 6.62 \times 10^{-5}$ h$^{-1}$ with $t_{1/2} = 10500$ h in dry sandy soil; $k = 2.55 \times 10^{-3}$ h$^{-1}$ in moist sandy loam (Graebing & Chib 2004)

Oxidation: photooxidation $t_{1/2} = 4.1$ h in air, estimated from the vapor-phase reaction with $5 \times 10^5$ hydroxyl radicals/m$^3$ in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

$k_{OH} = 9.7 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K in gas phase with atmospheric lifetime of 4.1 h but reduced to .19 h at 283 K; log $k_{OH(aq.)} = 8.2 \times 10^9$ M$^{-1}$ s$^{-1}$ in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis:

$k$(acid) = $2.1 \times 10^{-2}$ M$^{-1}$ s$^{-1}$ for acid catalyzed hydrolysis, $k$(neutral) = $4.3 \times 10^{-4}$ M$^{-1}$ s$^{-1}$ for neutral hydrolysis and $k$(alkaline) = $5.3 \times 10^{-3}$ M$^{-1}$ s$^{-1}$ for base catalyzed hydrolysis with $10^{-5}$ M in aqueous buffer (Faust & Gomaa 1972; quoted, Freed 1986; Harris 1982)

$t_{1/2} = 11.77$ h at pH 3.1, $t_{1/2} = 185$ d at pH 7.4 and $t_{1/2} = 6.0$ d at pH 10.4 in water at 20°C (Worthing & Hance 1991; Tomlin 1994)

$t_{1/2} = 11.77$ h at pH 3.1, $t_{1/2} = 185$ d at pH 7.4, $t_{1/2} = 136$ d at pH 9.0, and $t_{1/2} = 6$ d at pH 10.4 at 20°C (Montgomery 1993).

Biodegradation:

half-lives $t_{1/2} = 4.91$ d at pH 3.1 and $t_{1/2} = 185$ d at pH 7.4 from river die-away tests (Gomaa et al. 1969; quoted, Scow 1982)

$t_{1/2} = 12.5$ wk in sterile soils and $t_{1/2} < 1$ wk in nonsterile soils; $t_{1/2} = 6.5$ wk in sterile sandy loam and $t_{1/2} = 2$ wk in nonsterile sandy loam (Miles et al. 1979; quoted, Howard 1991)

$t_{1/2} = 32$ d in 0–10 cm depth of soil by 100 d leaching screening test (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

$k = 0.023$ d$^{-1}$ with estimated first-order $t_{1/2} = 30$ d in soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982)

$k$(av.) = 0.0193 d$^{-1}$ in silty clay with $t_{1/2} = 36$ d; and $k$(av.) = 0.0245 d$^{-1}$ in sandy clay with $t_{1/2} = 28$ d (Sattar 1990)

Biotransformation:

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

$k_2 = 0.070$ h$^{-1}$ (willow shiner, Tsuda et al. 1989)
$k_2 = 0.023$ h$^{-1}$ (eel’s liver, Sancho et al. 1993)
$k_2 = 0.019$ h$^{-1}$ (eel’s muscle, Sancho et al. 1993)
$k_2 = 0.21$ h$^{-1}$ (killifish Oryzias latipes, Tsuda et al. 1995)

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 4.1$ h, estimated from the vapor-phase reaction with $5 \times 10^5$ hydroxyl radicals/m$^3$ in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

Surface water: photolysis $t_{1/2} = 41$ d without humic substances; $t_{1/2} = 13$ d and $t_{1/2} = 5$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994);

$t_{1/2} = 144$ d at 6°C, $t_{1/2} = 69$ d at 22°C in darkness for Milli-Q water; $t_{1/2} = 181$ d at 6°C, $t_{1/2} = 80$ d at 22°C in darkness, $t_{1/2} = 43$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 132$ d at 6°C, $t_{1/2} = 52$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 125$ d at 6°C, $t_{1/2} = 50$ d at 22°C in darkness, $t_{1/2} = 47$ d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment: first-order degradation $k = 0.048$ d$^{-1}$ with $t_{1/2} = 14.4$ d under aerobic conditions, $k = 0.022$ d$^{-1}$ with $t_{1/2} = 31.7$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.033$ d$^{-1}$ with $t_{1/2} = 21.1$ d under aerobic conditions, $k = 0.029$ d$^{-1}$ with $t_{1/2} = 23.7$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2} = 43.8$ d in sterile soil at pH 4.7 (Sethunathan & MacRae 1969; quoted, Montgomery 1993); estimated persistence of 12 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
persistence of 3 months (Waughop 1978);
t_{1/2} = 12.5 wk in sterile sandy loam and t_{1/2} < 1.0 wk in nonsterile sandy loam; t_{1/2} = 6.5 wk in sterile organic soil and t_{1/2} = 2.0 wk in nonsterile organic soil (Miles et al. 1979);
estimated first-order t_{1/2} = 30 d in soil from biodegradation rate constant k = 0.023 d^{-1} for soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982);
moderate persistent in soil with t_{1/2} = 20–100 d (Willis & McDowell 1982);
t_{1/2} = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);
dissipation t_{1/2} = 19 d in soil (Glotfelty et al. 1990);
av. degradation rate constant k = 0.0193 d^{-1} in silty clay with t_{1/2} = 36 d and average degradation rate constant
k = 0.0245 d^{-1} in sandy clay with t_{1/2} = 28 d (Sattar 1990)
selected field t_{1/2} = 40 d (Waughop et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);
soil t_{1/2} = 65 d (Pait et al. 1992)
t_{1/2} = 40 d (selected, Halfon et al. 1996)
On sandy soil: first-order rate constants for photolytic decline, k = 5.45 \times 10^{-3} h^{-1} with t_{1/2} = 130 h irradiated in moisture-maintained soil, k = 0.84 \times 10^{-3} h^{-1} with t_{1/2} = 830 h irradiated in air-dried soil, k = 3.06 \times 10^{-3} h^{-1} with t_{1/2} = 230 h in dark control moist soil and k = 0.77 \times 10^{-3} h^{-1} with t_{1/2} = 900 h in dark control air-dried sandy soil from Sauk County, WI. The photolytic k = 2.39 \times 10^{-3} h^{-1} with t_{1/2} = 290 h in moist soil, k = 6.62 \times 10^{-5} h^{-1} with t_{1/2} = 10500 h in dry soil. The contribution of moisture to irradiated metabolism k = 4.61 \times 10^{-3} h^{-1} with t_{1/2} = 150 h, but for dark control system for k = 2.29 \times 10^{-5} h^{-1} with t_{1/2} = 300 h (Graebing & Chib 2004)
On sandy loam soil: first-order rate constants for photolytic decline, k = 4.07 \times 10^{-3} h^{-1} irradiated in moisture-maintained soil, k = 1.07 \times 10^{-3} h^{-1} irradiated in air-dried soil, k = 1.52 \times 10^{-3} h^{-1} in dark control moist soil and no degradation in dark control air-dried sandy loam soil from Madia, CA. t_{1/2} = 120 h for the first 96 h irradiation; over all t_{1/2} = 200 h from 96–168 h but in dark control system t_{1/2} = 460 h in moist sandy loam soil; irradiated metabolism t_{1/2} = 650 h in dry sandy loam soils. Rate constants due to photolysis k = 2.55 \times 10^{-3} h, and due to moisture k = 3.0 \times 10^{-3} h in moist sandy loam soil (Graebing & Chib 2004)
Biota: biochemical t_{1/2} = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);
excretion t_{1/2} = 9.9 h by willow shiner (Tsuda et al. 1989)
t_{1/2} = 25 h in eel’s liver and t_{1/2} = 26 h in eel’s muscle (Sancho et al. 1993)
### TABLE 18.1.1.27.1
Reported vapor pressures and Henry’s law constants of diazinon at various temperatures

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<th></th>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
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<tbody>
<tr>
<td></td>
<td>Vapor pressure</td>
<td>Henry’s law constant</td>
</tr>
<tr>
<td></td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td></td>
<td>P/mmHg</td>
<td>t/°C</td>
</tr>
<tr>
<td>Kim et al. 1984, Kim 1985</td>
<td>25.3 0.0113</td>
<td>25 0.014</td>
</tr>
<tr>
<td></td>
<td>34.9 0.0299</td>
<td>50 0.22</td>
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<tr>
<td></td>
<td>45.0 0.0770</td>
<td>75 2.20</td>
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<tr>
<td></td>
<td>20.0 0.0064</td>
<td>100 17.0</td>
</tr>
<tr>
<td></td>
<td>25.0 0.0109</td>
<td>125 100</td>
</tr>
</tbody>
</table>

\[
\log P = A - \frac{B}{(T/K)}
\]

\[
\log P = A - \frac{B}{(T/K)}
\]

A 9.3871 13.482 293.15 0.0349
B 4014.67 4571.2 293.15 0.0375

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

H’/(M/atm)
A –32.5647
B 11900

**FIGURE 18.1.1.27.1** Logarithm of vapor pressure versus reciprocal temperature for diazinon.
FIGURE 18.1.1.27.2 Logarithm of Henry's law constant versus reciprocal temperature for diazinon.
18.1.1.28 Dichlorvos

Common Name: Dichlorvos


Chemical Name: 2,2-dichlorovinyl-\(O,O\)-dimethyl phosphate; 2,2-dichloroethenyl-\(O,O\)-dimethyl phosphate

Uses: insecticide and fumigant to control flies, mosquitoes, and moths; also used as acaricide.

CAS Registry No: 62-73-7

Molecular Formula: \(C_4H_7Cl_2O_4P\)

Molecular Weight: 220.976

Melting Point (°C):
- Colorless to amber liquid (Hartley & Kidd 1987)

Boiling Point (°C):
- 35, 74, 117 (at 0.05, 1.0, 10 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)
- 234.1 (Tomlin 1994)

Density (g/cm\(^3\) at 20°C):
- 1.425 (Tomlin 1994)
- 1.440 (Montgomery 1993)

Molar Volume (cm\(^3\)/mol):
- 167.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, \(pK_a\):

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: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
- 10000 (Günther et al. 1968; Melnikov 1971; Kenaga 1980a; Khan 1980; Spencer 1982)
- 10000 (Martin & Worthing 1977; Worthing 1979; Worthing & Walker 1987)
- 16000 (Kawamoto & Urano 1989)
- 16000 (20°C, Montgomery 1993)
- 8000 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 1.60 (20°C, Eichler 1965; Wolfdietrich 1965)
- 1.60 (20°C, Melnikov 1971; Hartley & Graham-Bryce 1980; Spencer 1982; Montgomery 1993)
- 1.60* (20°C, evaporation rate-gravimetric method, measured range 293–333 K, Gückel et al. 1973)
- 1.60 (Khan 1980; Brouwer et al. 1994)

\[
\log (P/mmHg) = 9.9081 - 3464/(T/K); \text{ temp range not specified (quoted from literature, Gückel et al. 1982)}
\]

\[
0.947^* (20^\circ C, \text{ evap rate-gravimetric method, measured range 20–60°C, Gückel et al. 1982})
\]

\[
7.026 (\text{ gas saturation-GC, Kim et al. 1984})
\]

\[
4.011 (20, 25°C, \text{ extrapolated-Clausius-Clapeyron eq., Kim et al. 1984})
\]
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<tr>
<th>Property</th>
<th>Value</th>
<th>Source and Notes</th>
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<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C)</td>
<td>0.67</td>
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<td>1.60, 3.90</td>
<td>(20°C, 30°C, Hartley &amp; Kidd 1987)</td>
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<td>7.0</td>
<td>(20°C, selected, Suntio et al. 1988)</td>
</tr>
<tr>
<td></td>
<td>0.29</td>
<td>(20°C, Worthing &amp; Hance 1991)</td>
</tr>
<tr>
<td></td>
<td>0.267</td>
<td>(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)</td>
</tr>
<tr>
<td></td>
<td>2.10</td>
<td>(Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>7.94</td>
<td>(gradient GC method; Tsuzuki 2000)</td>
</tr>
<tr>
<td></td>
<td>6.92; 8.51, 5.62</td>
<td>(gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log K&lt;sub&gt;ow&lt;/sub&gt;</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.40</td>
<td>(Leo et al. 1971; Hansch &amp; Leo 1979)</td>
</tr>
<tr>
<td></td>
<td>2.29</td>
<td>(Rao &amp; Davidson 1980)</td>
</tr>
<tr>
<td></td>
<td>1.47</td>
<td>(shake flask-GC, Bowman &amp; Sans 1983)</td>
</tr>
<tr>
<td></td>
<td>1.16</td>
<td>(HPLC-RT correlation, Kawamoto &amp; Urano 1989)</td>
</tr>
<tr>
<td></td>
<td>1.40–2.29</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td></td>
<td>1.73</td>
<td>(RP-HPLC-RT correlation, Sicbaldi &amp; Finizio 1993)</td>
</tr>
<tr>
<td></td>
<td>1.43</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td></td>
<td>1.90</td>
<td>(Tomlin 1994)</td>
</tr>
<tr>
<td></td>
<td>1.42</td>
<td>(selected, Hansch et al. 1995)</td>
</tr>
<tr>
<td></td>
<td>1.73</td>
<td>(RP-HPLC-RT correlation, Finizio et al. 1997)</td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF</td>
<td>0.477</td>
<td>(calculated-S, Kenaga 1980a; quoted, Howard 1991)</td>
</tr>
<tr>
<td></td>
<td>~0.097</td>
<td>(whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992; quoted, Devillers et al. 1996)</td>
</tr>
<tr>
<td></td>
<td>~0.30</td>
<td>(whole body carp, Tsuda et al. 1993)</td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log K&lt;sub&gt;oc&lt;/sub&gt;</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.45</td>
<td>(soil, calculated-S, Kenaga 1980a; quoted, Howard 1991)</td>
</tr>
<tr>
<td></td>
<td>1.67</td>
<td>(correlated, Kawamoto &amp; Urano 1989)</td>
</tr>
<tr>
<td></td>
<td>1.70</td>
<td>(calculated, Montgomery 1993)</td>
</tr>
<tr>
<td></td>
<td>1.67; 2.98, 2.04</td>
<td>(soil, quoted exp;: estimated-class-specific model, estimated-general model, Gramatica et al. 2000)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k, or Half-Lives, <i>t</i><sub>½</sub>:

Volatilization: based on the Henry's law constant, <i>t</i><sub>½</sub> ~ 57 d from a model river (Lyman et al. 1982; quoted, Howard 1991);

<math> t_{½} \sim 400 \text{ yr} \text{ from an model pond, which considered the effect of adsorption (Howard 1991).} \end{math>

Photolysis:

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: atmospheric <i>t</i><sub>½</sub> = 320 d, based on an estimated rate constant k<sub>O3</sub> = 3.58 × 10<sup>–20</sup> cm<sup>3</sup>·molecule<sup>–1</sup>·s<sup>–1</sup> at 25°C for the vapor-phase reaction with ozone of concn 7 × 10<sup>13</sup>/cm<sup>3</sup> in air (Atkinson & Carter 1984; quoted, Howard 1991)
Insecticides

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k_{OH} = 9.24 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^{5}$/cm$^3$ in air (Atkinson 1987; quoted, Howard 1991).

$k_{OH} = 9.4 \times 10^{-12}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ with calculated tropospheric lifetime about 1.2 d at 298 K assuming an average OH concn of $1 \times 10^6$ molecule/cm$^3$ (Gautier et al. 2003)

Hydrolysis: $t_{1/2} = 462$ min at pH 7 and $t_{1/2} = 30$ min at pH 8 (Montgomery 1993);

$1/2 \approx 31.9$ d at pH 4, $t_{1/2} \approx 2.9$ d at pH 7, and $t_{1/2} \approx 2.0$ d at pH 9 at 22°C (Tomlin 1994)

$1/2 = 3800$ d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: the presence of active microorganisms reduced the $t_{1/2}$ to 0.9–0.75 and 0.85 to 0.70 d in autoclaved clay and calcareous soil, respectively (Guirguis & Shafik 1975; quoted, Howard 1991);

rate constant $k$(aerobic) = 0.20 d$^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by aerobic activated sludge, and $k$(anaerobic) = 0.20 d$^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

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

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 320$ d, based on an estimated rate constant $k = 3.58 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C for the vapor-phase reaction with ozone of $7 \times 10^{11}$/cm$^3$ in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k = 2.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^{5}$/cm$^3$ in air (Atkinson 1987; quoted, Howard 1991)

atmospheric transformation lifetime was estimated to be $<1$ d (Kelly et al. 1994)

Calculated tropospheric lifetime of 0.5 d for reaction with OH radicals, wet deposition lifetime estimated to be 5.6 d in the atmosphere by rainfall (Gautier et al. 2003)

Surface water: half-lives in lakes and rivers are reported to be approximately 4 d (Lamoreaux & Newland 1978; quoted, Howard 1991)

Biodegradation $t_{1/2} = 3.5$ d by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)

Biodegradation $t_{1/2}$(aerobic) = 180 d, $t_{1/2}$(anaerobic) = 1 d, hydrolysis $t_{1/2} = 3800$ d at pH 7 in natural waters (Capel & Larson 1995)

Ground water:

Sediment:

Soil: average degradation rate constant $k = 0.0423$ d$^{-1}$ in silty clay with $t_{1/2} = 16$ d and average degradation rate constant $k = 0.0444$ d$^{-1}$ in sandy clay with $t_{1/2} = 16$ d (Sattar 1990);

selected field $t_{1/2} = 0.5$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
<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 m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.60</td>
<td>20</td>
<td>0.947</td>
<td>10</td>
<td>0.00322</td>
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<tr>
<td>30</td>
<td>4.0</td>
<td>40</td>
<td>7.30</td>
<td>11</td>
<td>0.00378</td>
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<tr>
<td>40</td>
<td>9.33</td>
<td>60</td>
<td>40.0</td>
<td>12</td>
<td>0.00504</td>
</tr>
<tr>
<td>50</td>
<td>-</td>
<td>12</td>
<td>0.00520</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>-</td>
<td>18</td>
<td>0.0109</td>
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<td>15</td>
<td>0.00209</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>20</td>
<td>0.00289</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22.5</td>
<td>0.0181</td>
<td></td>
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</tr>
<tr>
<td>23</td>
<td>0.0230</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.0230</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.0247</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>0.0289</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>0.0253</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Arrhenius expression:
\[
\ln H/(\text{M atm}^{-1}) = -A + B/(T/K)
\]

A = 28.904
B = 11100

**FIGURE 18.1.1.28.1** Logarithm of vapor pressure versus reciprocal temperature for dichlorvos.
**FIGURE 18.1.1.28.2** Logarithm of Henry's law constant versus reciprocal temperature for dichlorvos.
18.1.1.29 Dicrotophos

Common Name: Dicrotophos

Synonym: Bidirl, Bidrin, C 709, Cabicron, Carbamicron, CIBA 709, Diapadrin, Dicrotosof, Ektafos, ENT 24,482, Karbicron, Shell SD-3562

Chemical Name: \((E)-2\text{-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate};\) \((E)-3\text{-}(diethylamino)-1\text{-methyl-3-oxo-1-propenyl dimethyl phosphate}\)

Uses: contact and systemic insecticide and acaricide to control pests on rice, cotton, maize, soybeans, coffee, citrus, and potatoes.

CAS Registry No: 141-66-2 \textit{cis}-dicrotophos

Molecular Formula: \(\text{C}_8\text{H}_{16}\text{NO}_5\text{P}\)

Molecular Weight: 237.191

Melting Point (°C): liquid

Boiling Point (°C):

\[130\] (at 0.1 mmHg, Worthing & Hance 1991; Montgomery 1993; Milne 1995)

\[400\] (Tomlin 1994; Milne 1995)

Density (g/cm³ at 20°C):

\[1.216\] (Hartley & Kidd 1987)

\[1.216\] (15°C, Merck Index 1989; Milne 1995)

\[1.21\] (technical grade, Worthing & Hance 1991)

\[1.216\] (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm³/mol):

Dissociation Constant, \(pK_a\):

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):

miscible (Spencer 1973)

miscible (Hartley & Kidd 1987; Budavari 1989; Milne 1995)

miscible (Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)


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):

\[0.0115^*\] (20°C, extrapolated, gas saturation-GC, measured range 32.3–77°C, Grayson & Fosbracey 1982)

\[
\ln (P/\text{Pa}) = 21.6 - 7631/(T/\text{K}); \text{ temp range 32.3–77°C, (Antoine eq., gas saturation-GC, Grayson & Fosbracey 1982)}
\]

\[0.0093\] (20°C, Hartley & Kidd 1987)

\[0.0093\] (20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

\[0.0213\] (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol at 25°C):

\(5.05 \times 10^{-6}\) (20–25°C, calculated-P/C)

Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):

\ [-0.260\] (calculated as per Broto et al. 1984, Karcher & Devillers 1990)

\ [-0.49\] (shake flask, Log P Database, Hansch & Leo 1987)

\ [-0.49\] (recommended, Sangster 1993)

\ [-0.50\] (Montgomery 1993)

\ [0.0\] (Hansch et al. 1995)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 1.04–2.27 (Montgomery 1993)
- 1.66 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.66; 1.49, 1.67 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Hydrolysis: $t_{1/2} = 117, 72, \text{ and } 28 \text{ d in buffer solutions of pH 5, 7, and 9, respectively, at 25°C (Lee et al. 1989; quoted, Montgomery 1993)}$;
  $\text{calculated } t_{1/2} = 88 \text{ d in water at 20°C at pH 5 and } = 23 \text{ d at pH 9 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).}$

Half-Lives in the Environment:
- Soil: $t_{1/2} = 3 \text{ d in sandy loam soil (Lee et al. 1989; quoted, Montgomery 1993)}$;
  $\text{selected field } t_{1/2} = 20 \text{ d (Wauchope et al. 1992; Hornsby et al. 1996).}$

### TABLE 18.1.1.29.1

Reported vapor pressures of dicrotophos at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>32.3</td>
<td>0.034</td>
</tr>
<tr>
<td>33.7</td>
<td>0.036</td>
</tr>
<tr>
<td>41.0</td>
<td>0.055</td>
</tr>
<tr>
<td>45.2</td>
<td>0.106</td>
</tr>
<tr>
<td>51.0</td>
<td>0.136</td>
</tr>
<tr>
<td>60.1</td>
<td>0.287</td>
</tr>
<tr>
<td>65.8</td>
<td>0.405</td>
</tr>
<tr>
<td>69.5</td>
<td>0.424</td>
</tr>
<tr>
<td>77.0</td>
<td>0.820</td>
</tr>
<tr>
<td>30</td>
<td>0.0115</td>
</tr>
</tbody>
</table>

\[
\ln P = A - B/(T/K)
\]

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>7631</td>
<td>21.6</td>
</tr>
</tbody>
</table>
**FIGURE 18.1.1.29.1** Logarithm of vapor pressure versus reciprocal temperature for dicrotophos.
18.1.1.30 Dieldrin

Common Name: Dieldrin
Synonym: Aldren, Alvit, Alyran, Compound 497, Dieldrite, Dieldrix, Dorotox, ENT 16225, HEOD, Illoxol, Insectlack, Kombi-Albertan, NA 2761, NCI-C00124, Octalox, Panoram D-31, Quintox
Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8, 8a-octahydroendo-1,4-exo-5,8-dimethano-naphthalene; 3,4,5,6,9,9-hexachloro-1a,2a,2a,3,6,6a,7,7a-octahydro-2,7,3,6-dimethanonaphth[2,3-b]oxirene
Uses: insecticide to control public health insect pests, termites, locusts, and tropical disease vectors.
CAS Registry No: 60-57-1
Molecular Formula: C_{12}H_{8}Cl_{6}O
Molecular Weight: 380.909
Melting Point (°C): 175.5 (Lide 2003)
Boiling Point (°C): 265, 352, 404 (estimated from structure, Tucker et al. 1983)
Density (g/cm³ at 20°C): 1.75 (Hartley & Kidd 1987; Montgomery 1993)
Molar Volume (cm³/mol): 318.2 (calculated-Le Bas method at normal boiling point)
253.6 (Ruelle & Kesselring 1997)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
76.6 (Rordorf 1989)
Enthalpy of Fusion, ΔH₅ₜₐₜ (kJ/mol):
21.4 (Rordorf 1989)
18.41 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS₅ₜₐₜ (J/mol K):
41.34, 48.12 (Plato 1972)
47 (Rordorf 1989)
44.77 (Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS₅ₜₐₜ = 56 K/mol K), F:
0.026 (20°C, Suntio et al. 1988)
0.033 (Mackay et al. 1986)
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):
0.19 (colorimetric method, Lipke & Kearns 1960)
0.25* (shake flask-GC/UV, measured range 25–45°, Richardson & Miller 1960)
0.14–0.18 (particle size of 0.04–5.0µ, shake flask-GC, Robeck et al. 1965)
0.15 (Eye 1968; quoted, Freed 1976; Jury et al. 1983,84)
0.20 (Günther et al. 1968)
0.186 (25–29°C, shake flask-GC/ECD, Park & Bruce 1968)
0.022 (Biggar & Riggs 1974)
0.195* (particle size of ≤ 0.5µ, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 & 5.0µ; shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
0.20 (generator column-GC/ECD, Weil et al. 1974)
0.187 (Martin & Worthing 1977; Worthing & Walker 1987)
0.10–0.25 (Wauchope 1978)
0.022 (Kenaga 1980a, b; Garten & Trabalka 1983; Isnard & Lambert 1989)
0.10 (Weber et al. 1980; Eadie & Robbins 1987)
0.468 (20–25°C, shake flask-GC, Kanazawa 1981)
0.19 (20°C, Hartley & Kidd 1987)
0.14, 0.20 (20°C, 30°C, Montgomery 1993)
0.20 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.57, 4.95 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

\[ \log \left[ \frac{C_L}{(\text{mol m}^{-3})} \right] = -1158/(T/K) + 1.94 \] (supercooled liquid, linear regression of literature data, 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):**

1.04 \times 10^{-4} (20°C, Porter 1964)
1.04 \times 10^{-4}, 1.91 \times 10^{-4}, 3.65 \times 10^{-4} (20, 30, 40°C, effusion method, Porter 1964 as quoted in Spencer & Cliath 1969)
2.4 \times 10^{-3} (Eichler 1965; Martin 1972; Melnikov 1971)
3.47 \times 10^{-4}, 1.33 \times 10^{-3}, 4.63 \times 10^{-3} (20, 30, 40°C, gas saturation method, Spencer & Cliath 1969)
6.59 \times 10^{-4} (calculated from vapor pressure eq. apparent vapor pressure, Spencer & Cliath 1969)

\[ \log (P/\text{mmHg}) = 12.07 - 5178/(T/K); \text{ for temp range 20–40°C (gas saturation, apparent vapor pressure, Spencer & Cliath 1969)} \]
6.77 \times 10^{-4} (gas saturation, Spencer & Cliath 1969)
3.87 \times 10^{-4} (20°C, partition coeff., Atkins & Eggleton 1971)
4.13 \times 10^{-4} (20°C, Khan 1980)
2.40 \times 10^{-3} (20–25°C, Weber et al. 1980)
8.90 \times 10^{-4} (20°C, GC, Seiber et al. 1981)
4.20 \times 10^{-4} (20°C, gas saturation-GC, extrapolated, measured range 35–75°C, Grayson & Fosbracey 1982)

\[ \ln (P/\text{Pa}) = 30.7 – 11285/(T/K); \text{ temp range 35 to 75.2°C (gas saturation-GC, Grayson & Fosbracey 1982)} \]
0.00532, 0.0597 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.0215 (supercooled liquid P_{L}, converted from literature P_{S} with ΔS_{fus} Bidleman 1984)
4.00 \times 10^{-4} (20°C, Hartley & Kidd 1987)
7.90 \times 10^{-4} (gas saturation-GC, measured range 25–125°C, Rordorf 1989)

\[ \log (P_{L}/\text{Pa}) = 14.37 – 5210.07/(T/K); \text{ measured range 32.4–125°C (solid, gas saturation-GC, Rordorf 1989)} \]
\[ \log (P_{S}/\text{Pa}) = 11.66013 – 4001.62/(T/K); \text{ temp range not specified (liquid, gas saturation-GC, Rordorf 1989)} \]
0.0215, 0.0101 (supercooled P_{L}, converted from literature P_{S} with different ΔS_{fus} values, Hinckley et al. 1990)
0.00532, 0.0318 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
\[ \log (P_{GC}/\text{Pa}) = 12.46 – 4310/(T/K) \] (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
2.37 \times 10^{-4} (20°C, Montgomery 1993)
4.00 \times 10^{-4} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.010 (supercooled liquid P_{L}, Wania & Mackay 1996)
3.24 \times 10^{-4} (liquid P_{L}, GC-RT correlation., Donovan 1996)
0.016, 0.014 (supercooled liquid P_{L}; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
\[ \log (P_{L}/\text{Pa}) = -3995/(T/K) + 11.62 \] (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

**Henry’s Law Constant (Pa·m^3/mol at 25°C):**

4.59 (gas stripping, Atkins & Eggleton 1971)
0.02 (calculated-P/C, Mackay & Leinonen 1975)
0.0171 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
5.84 (exptl., Warner et al. 1980)
0.0456 (calculated-P/C, Levens 1981)
1.10 (20°C, Mackay & Shiu 1981)
2.94 (20°C, measured, Slater & Spedding 1981)
0.172 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
0.78 (calculated-P/C, Mackay et al. 1986)
Insecticides

0.74  (WERL Treatability Database, quoted, Ryan et al. 1988)
1.12  (20°C, calculated-P/C, Suntio et al. 1988)
1.0   (calculated-P/C, Nash 1989)
5.88  (Montgomery 1993)
1.016 (wetted wall column-GC, Altschuh et al. 1999)
1.0, 1.1 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 2.60  (Hansch & Leo 1979)
- 5.48  (calculated, Kenaga 1980a, b)
- 6.20  (TLC-retention time correlation, Lord et al. 1980)
- 4.32  (shake flask-GC, Kanazawa 1981)
- 6.20  (20°C, shake flask-GC, Briggs 1981)
- 5.11  (HPLC-RT correlation, Hammers et al. 1982)
- 5.30  (RP-HPLC correlation, Hermens & Leeuwangh 1982)
- 5.10  (shake flask-GC, Platford 1982)
- 4.32  (Hansch & Leo 1985; Medchem Database 1988)
- 4.51, 4.49, 4.60, 4.55 (shake flask, Brooke et al. 1986)
- 4.51  (HPLC-RT correlation, De Kock & Lord 1987)
- 5.40  (shake flask/slow-stirring method, De Bruijn et al. 1989)
- 3.69–6.20 (Montgomery 1993)
- 4.76  (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 5.20  (selected, Hansch et al. 1995)
- 4.76  (RP-HPLC-RT correlation, Finizio et al. 1997)
- 5.40, 5.58 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
- 7.40  (calculated-$K_{ow}/K_{aw}$, Wania & Mackay 1996)
- log $K_{oa} = -3.82 + 3790/(T/K)$, temp range: 5–45°C (gas saturation-GC, Shoeib & Harner 2002)
- 8.89, 8.84 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
- 3.08, 4.14, 4.69 (algae, daphnia, guppies, Reinert 1967)
- 3.65–4.69 (earthworms, Wheatley & Hardman 1968)
- 0.230 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Robinson et al. 1969)
- 0.322 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Walker et al. 1969)
- 3.04–3.66 (Saccharomyces cerevisiae, Voerman & Tammes 1969)
- 3.0–5.48 (benthic algae, Rose & McIntire 1970)
- 0.301 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Baron & Walton 1971)
- 3.24 (soft clam, Butler 1971)
- 3.11, 3.54, 2.37 (Scenedesmus obliquus, Daphnia magna, Reinert 1972)
- 2.37 (water basis, Scenedesmus obliquus, Reinert 1972)
- 3.43, 4.79, 2.66–4.60 (Gambusia, Physa, Oedogonium sp., Metcalf et al. 1973)
- 4.51 (water basis, Ankistrodesmus, Neudorf & Khan 1975)
- 3.39 (oyster, Mason & Rowe 1976)
- 3.20 (mussel, steady state, Ernst 1977)
- 2.30 (Anabaena cylindrica, Schauerger & Wildman 1977)
- 2.70; 3.26 (Anacystis nidulans, Nostoc muscorum, Schauerger & Wildman 1977)
- 2.0–4.0 (Callahan et al. 1979; quoted, Howard 1991)
- 3.76, 3.65 (fish: flowing water, static water; Kenaga 1980a, b; Kenaga & Goring 1980)
- 0.362 (average beef fat diet, Kenaga 1980b)
- 3.54 (pulex, Kenaga & Goring 1980)
- 3.62 (earthworms, Lord et al. 1980)

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2.00  
(\textit{Triaenodes tardus}, Belluck & Felsot 1981)

3.65  
(\textit{Pseudorasbora parva}, flow-through conditions, Kanazawa 1981)

1.0–5.0  
(selected, Schnoor & McAvoy 1981)

3.37  
(mussel, quoted average, Geyer et al. 1982)

4.23–4.98  
(earthworms, Gish & Hughes 1982)

4.16  
(fish, correlated, Mackay 1982)

3.52  
(trout, Verschuuren 1983)

3.55  
(clam fat, 60-d expt., Hartley & Johnson 1983)

4.10  
(guppy, Davies & Dobbs 1984)

4.25  
(activated sludge, Freitag et al. 1984)

3.36, 3.48, 4.25  
(algae, golden ide, activated sludge, Freitag et al. 1985)

3.33, 3.29  
(mussel, calculated values, Zaroogian et al. 1985)

3.33, 3.29  
(oyster, calculated values, Zaroogian et al. 1985)

3.70, 3.90  
(oyster, quoted from Zaroogian et al. 1985; Hawker & Connell 1986)

1.72–1.95  
(human fat lipid basis, Geyer et al., 1987)

1.56–1.78  
(human fat wet wt. basis, Geyer et al., 1987)

4.10  
(quoted, Isnard & Lambert 1988; Howard 1991)

–2.10  
(beef biotransfer factor log B_b, correlated-KOW, Potter et al. 1974)

–1.97  
(milk biotransfer factor log B_m, correlated-KOW, Saha 1969; Wilson & Cook 1972)

–1.01  
(vegetation, correlated-\textit{K}_{\text{ow}}, Beall & Nash 1972; quoted, Travis & Arms 1988)

2.96–4.11  
(aquatic food web, Fordham & Reagan 1991)

3.81  
(fish, Fordham & Reagan 1991)

3.88  
(selected, Chessells et al. 1992)

3.36, 4.06  
(algae \textit{Chlorella}: wet wt basis, dry wt basis, Geyer et al. 2000)

3.49, 5.49  
(mussel \textit{Mytilus edulis}: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.54, 5.57  
(\textit{Daphnia}: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.46, 5.54  
(oyster \textit{Crassostrea virginica}: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.32, 5.34  
(oyster \textit{Crassostrea virginica}: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.70, 5.62  
(oyster \textit{Crassostrea virginica}: wet wt basis, lipid wt basis, Geyer et al. 2000)

4.10, 5.26  
(guppy female: wet wt basis, lipid wt basis, Geyer et al. 2000)

4.41, 5.41  
(carp: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.32, 5.34  
(oyster \textit{Crassostrea virginica}: wet wt basis, lipid wt basis, Geyer et al. 2000)

1.69; 1.85  
(human: wet wt basis, lipid wt basis, Geyer et al. 2000)

3.65; 3.66  
(\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 \textit{K}_{\text{OC}}:}

4.55  
(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)

4.08  
(calculated-\textit{K}_{\text{OW}}, Rao & Davidson 1980)

3.87  
(extrapolated from RP-TLC and reported as log \textit{K}_{\text{OM}}, Briggs 1981)

4.0  
(selected, Schnoor & McAvoy 1981; Schnoor 1992)

3.36–3.85  
(reported as log \textit{K}_{\text{OM}}, Mingelgrin & Gerstl 1983)

4.08  
(soil, screening model calculations, Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)

4.36  
(calculated-\textit{K}_{\text{OW}} as per Kenaga & Goring 1980, Chapman 1989)

4.15  
(soil: clay loam/kaolinite, 20°C, batch equilibrium-sorption isotherm, Kishi et al. 1990)

4.50  
(sediment, Fordham & Reagan 1991)

4.10  
(soil, quoted exptl., Meylan et al. 1992)

4.03  
(soil, calculated-MCI \chi and fragment contribution, Meylan et al. 1992)

5.08  
(estimates-QSAR and SPARC, Kollig 1993)

4.08–4.55  
(Montgomery 1993)

4.08  

4.55  
(soil, calculated-MCI \chi, Sabljic et al. 1995)

4.71  
(soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)

4.90; 4.10  
(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

4.08; 4.06  
(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatileization: $t_{\text{vol}} \sim 1.4$ d from a model river of depth 1 m flowing at 1 m/s with a wind velocity of 3 m/s by using Henry’s law constant (Lyman et al. 1982; quoted, Howard 1991).

Photolysis: rate constant $k = 4.8 \times 10^{-4}$ h−1 by direct sunlight at 40° latitude (Mabey et al. 1982); using fungus and 254 nm UV, more than 90% initial added amounts were degraded in 4 weeks of incubation (Katayama & Matsumura 1991).

Oxidation: rate constant for singlet oxygen, $k < 3600$ M−1 h−1 and for RO2 radicals $k < 30$ M−1 h−1 (Mabey et al. 1982); photooxidation $t_{\text{ox}} = 4–40.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); calculated tropospheric lifetimes of 1.1 d due to gas-phase reaction with OH radical (Atkinson et al. 1992).

Hydrolysis: first-order $t_{\text{hyd}} = 10.5$ yr based on a first-order rate constant $k = 7.5 \times 10^{-6}$ h−1 at pH 7.0 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993); rate constant $k = 6.3 \times 10^{-2}$ yr−1 at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{\text{b,aq}} = 4200–25,920$ h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Howard 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991); $t_{\text{b,aq}} = 868$ d (Nash 1980; quoted, Jury et al. 1983); rate constant $k = 0.013$ d−1 from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982); aqueous anaerobic $t_{\text{b,an}} = 24–168$ h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991); $t_{\text{b,an}} = 870$ d in soil by 100-d leaching screening simulation in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989).

Biotransformation:

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

$k_1 = 20.40$ h−1; $k_2 = 0.013$ h−1 (Ernst 1977; quoted, Hawker & Connell 1986)

$k_2 = 0.017$ d−1 (fish, Fordham & Reagan 1991)

$k_2 = 0.014$ d−1 (birds, Fordham & Reagan 1991)

Half-Lives in the Environment:

Air: $t_{\text{air}} = 4–40.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995); calculated life-time of 1.1 d in troposphere (Atkinson et al. 1992).

Surface water: estimated $t_{\text{sw}} \geq 300$ d in lake waters (Zoeteman et al. 1980);

$t_{\text{sw}} = 4200–25920$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991; quoted, Mortimer & Connell 1995).

Ground water: $t_{\text{gw}} = 24–51840$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{\text{s,d}} = 15100$ h (mean value quoted from Howard et al. 1991).

Soil: field $t_{\text{f,s}} = 49$ d in nondisked soil (Nash 1983);

$\sim 7$ yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 3 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{\text{f,s}} = 4200–25920$ h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991); “best estimate” of 10 yr for 95% disappearance, the “true value” lies between 8.2–13.6 yr in experimental field (Freeman et al. 1975);

persistence of more than 36 months (Wauchope 1978);

first-order $t_{\text{f,s}} \sim 53.3$ d from rate constant $k = 0.013$ d−1 from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{\text{s,d}} = 20–100$ d (Willis & McDowell 1982);

microagroecosystem $t_{\text{s,d}} = 19–26$ d in moist fallow soil (Nash 1983);

measured dissipation rate $k = 0.055$ d−1 (Nash 1983; quoted, Nash 1988);

estimated dissipation rate $k = 0.034$ and 0.049 d−1 (Nash 1988);
biodegradation $t_{1/2} = 868$ d (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
t$1/2 > 50$ d and subject to plant uptake via volatilization (Ryan et al. 1988);
estimated field $t_{1/2} = 1000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{1/2} = 5$ – 9 yr in soil (Geyer et al. 2000)
t$1/2 = 21.7$ and $25$ yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: estimated $t_{1/2} = 1.3$ and $10.2$ d in rat’s liver, and similar values estimated $t_{1/2} = 10.3$ d for the blood in rat and $t_{1/2} = 3$ d in adipose tissue of rat (Robinson et al. 1969);
t$1/2 = 53.1$ h in mussels (Ernst 1977; quoted, Hawker & Connell 1986);
biomathematical $t_{1/2} = 868$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989)

### TABLE 18.1.1.30.1
Reported aqueous solubilities and octanol-air partition coefficients of dieldrin at various temperatures

<table>
<thead>
<tr>
<th>Richardson &amp; Miller 1960</th>
<th>Biggar &amp; Riggs 1974</th>
<th>Shoeib &amp; Harner 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-UV spec.</td>
<td>shake flask-GC</td>
<td>generator column-GC/MS</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>25</td>
<td>0.25</td>
<td>15</td>
</tr>
<tr>
<td>35</td>
<td>0.54</td>
<td>25</td>
</tr>
<tr>
<td>45</td>
<td>1.0</td>
<td>35</td>
</tr>
<tr>
<td>45</td>
<td>0.090</td>
<td>45</td>
</tr>
</tbody>
</table>

log $K_{OA} = A + B/(T/K)$

$A = -3.82$

$B = 3790$

enthalpy of phase change

$\Delta H_{OA}/(kJ mol^{-1}) = 72.6$

### FIGURE 18.1.1.30.1
Logarithm of mole fraction solubility ($ln x$) versus reciprocal temperature for dieldrin.
FIGURE 18.1.1.30.2 Logarithm of $K_{OA}$ versus reciprocal temperature for dieldrin.

<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>wet</td>
<td></td>
<td></td>
<td></td>
<td>set 1</td>
<td>set 2</td>
</tr>
<tr>
<td>20</td>
<td>$3.47 \times 10^{-4}$</td>
<td>35.0</td>
<td>0.0026</td>
<td>25</td>
<td>0.00079</td>
</tr>
<tr>
<td>30</td>
<td>$1.32 \times 10^{-3}$</td>
<td>38.2</td>
<td>0.0042</td>
<td>50</td>
<td>0.018</td>
</tr>
<tr>
<td>40</td>
<td>$4.68 \times 10^{-3}$</td>
<td>51.5</td>
<td>0.017</td>
<td>75</td>
<td>0.25</td>
</tr>
<tr>
<td>dry</td>
<td></td>
<td></td>
<td></td>
<td>100</td>
<td>2.60</td>
</tr>
<tr>
<td>20</td>
<td>$3.73 \times 10^{-4}$</td>
<td>70.0</td>
<td>0.114</td>
<td>125</td>
<td>19.0</td>
</tr>
<tr>
<td>30</td>
<td>$1.35 \times 10^{-3}$</td>
<td>75.2</td>
<td>0.182</td>
<td>125</td>
<td>18.0</td>
</tr>
<tr>
<td>40</td>
<td>$4.52 \times 10^{-3}$</td>
<td>20</td>
<td>0.00042</td>
<td>eq. 1</td>
<td>$P_{s}/Pa$</td>
</tr>
<tr>
<td>eq.1</td>
<td>P/mmHg</td>
<td>eq. 1a</td>
<td>P/Pa</td>
<td>A</td>
<td>14.37</td>
</tr>
<tr>
<td>A</td>
<td>12.07</td>
<td>A</td>
<td>11285</td>
<td>B</td>
<td>5210.07</td>
</tr>
<tr>
<td>B</td>
<td>5178</td>
<td>B</td>
<td>30.7</td>
<td>eq. 1</td>
<td>$P_{l}/Pa$</td>
</tr>
<tr>
<td>A</td>
<td>11.6603</td>
<td>A</td>
<td>9.519590</td>
<td>B</td>
<td>4001.62</td>
</tr>
<tr>
<td>$\Delta H_v = 76.6$ kJ/mol</td>
<td>$\Delta H_v = 62.8$ kJ/mol</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 18.1.1.30.3 Logarithm of vapor pressure versus reciprocal temperature for dieldrin.
18.1.1.31 Diflubenzuron

Common Name: Diflubenzuron
Synonym: Deflubenzon, difluron, Dimilin, DU 112307, Duphacid, ENT 29054, OMS 1804, Largon, Micromite, PDD 60401, PH 60–40, TH-6040
Chemical Name: 1-(4-chlorophenyl)-3-(2,6-difluorobenzol) urea; N-[(4-chlorophenyl)-amino]carbonyl]-2,6-difluorobenzamide
Uses: nonsystemic insecticide to control leaf-eating larvae and leaf miners in forestry, woody ornamentals and fruit trees.
CAS Registry No: 35367-38-5
Molecular Formula: \( C_{14}H_{9}ClF_{2}N_{2}O_{2} \)
Molecular Weight: 310.683
Melting Point (°C):
230–232 (dec., Tomlin 1994)
239 (Lide 2003)
Boiling Point (°C):
dec. on distillation (Montgomery 1993)
Density (g/cm³ at 20°C):
288.3 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
Dissociation Constant, \( pK_a \):
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: 0.00795 (mp at 239°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.25 (Ivie et al. 1980; quoted, Belluck & Felsot 1981)
0.20 (Spencer 1982; Wauchope 1989)
0.14 (20°C, Hartley & Kidd 1987; Milne 1995)
0.10 (20°C, Worthing & Walker 1987, 1991)
14.0 (Montgomery 1993)
0.30 (Milne 1995)
0.08 (selected, Lohninger 1994)
0.08 (20–25°C, selected, Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
< 3.3 × 10⁻⁵ (50°C, Hartley & Kidd 1987)
< 1.3 × 10⁻⁵ (Worthing & Hance 1991)
3.33 × 10⁻⁵ (20°C, Montgomery 1993)
1.20 × 10⁻⁷ (gas saturation method, Tomlin 1994)
1.20 × 10⁻⁷ (20–25°C, selected, Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
4.70 × 10⁻⁴ (20–25°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
5.06 (Belluck & Felsot 1981)
3.88 (shake flask-UV, Sotomatsu et al. 1987)
2.12 (shake flask-UV, Nakagawa et al. 1991)
3.10 (selected, Nendza 1991)
3.29 (calculated, Montgomery 1993)
3.89 (Tomlin 1994)

Bioconcentration Factor, log BCF:
2.88 (calculated-S as per Kenaga & Goring, this work)
2.44 (calculated-$K_O$ as per Kenaga & Goring, this work)

Sorption Partition Coefficient, log $K_{OC}$:
3.01 (calculated, Montgomery 1993)
4.00 (average value, Dowd et al. 1993)
4.00 (20–25°C, selected, Hornsby et al. 1996)
4.06 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: half-lives at 20°C: $t_{1/2} > 150$ d at pH 5 and 7 and $t_{1/2} = 42$ d at pH 9 (Tomlin 1994).
$t_{1/2} > 300$ d at pH 2, $t_{1/2} = 100$ d at pH 7 and $t_{1/2} = 0.48$ d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)
Biodegradation: $t_{1/2}$ (aerobic) = 3 d, $t_{1/2}$ (anaerobic) = 12 d in natural waters (Capel & Larson 1995)
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: stable at pH 5 and 7 with $t_{1/2} > 150$ d, and $t_{1/2} = 42$ d at pH 9 and 20°C (Tomlin 1994)
biodegradation $t_{1/2}$ (aerobic) = 3 d, $t_{1/2}$ (anaerobic) = 12 d, hydrolysis $t_{1/2} > 300$ d at pH 2, $t_{1/2} = 100$ d at pH 7
and $t_{1/2} = 0.48$ d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Ground water:

Sediment:
Soil: $t_{1/2} < 7$ d (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);
$t_{1/2} = 10$ d in forest soil (Dowd et al. 1993);
field $t_{1/2} = 10$ d (20–25°C, selected, Hornsby et al. 1996).

Biota:
18.1.1.32 Dimethoate

Chemical Structure:

Common Name: Dimethoate

Chemical Name: \( O,O'-\text{dimethyl } S\text{-methylcarbamoyl-methyl phosphorodithioate; } O,O'-\text{dimethyl } S\text{-}(N\text{-monomethyl)car-bamylmethyl dithiophosphate; } 2\text{-dimethoxyphosphinothiolthio-N-methylacetamide}\)

Uses: systemic and contact insecticide to control thrips and red spider mites on many agricultural crops, sawflies on apples and plums, also wheat bulb and olive flies.

CAS Registry No: 60-51-5
Molecular Formula: \( \text{C}_5\text{H}_{12}\text{NO}_3\text{PS}_2 \)
Molecular Weight: 229.258

Melting Point (°C):
- 51–52 (Hartley & Kidd 1987)
- 49.0 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 52 (Lide 2003)

Boiling Point (°C):
- 107 (at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)
- 117 (at 0.1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
- 117 (tech. grade at 0.1 mmHg, Worthing & Hance 1991)

Density (g/cm³ at 20°C):
- 1.281 (50°C, Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):
- 205.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, \( pK_a \):

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
- 23.43 (DSC method, Plato & Glasgow 1969)

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: 0.543 (mp at 52°C)

Water Solubility (g/m³ or mg/L at 25°C at normal boiling point):
- 39000 (Melnikov 1971)
- 25000 (Martin & Worthing 1977; Worthing 1979; Kenaga 1980a)
- 25140 (Briggs 1981)
- > 5000 (20°C, shake flask-GC, Bowman & Sans 1983a)
- 25020 (20°C, shake flask-GC, Bowman & Sans 1983b)
- 25000 (22°C, Verschueren 1983)
- 25120 (Kanazawa 1989)
- 23300, 23800, 25000 (20°C, at pH 5, 7, 9, Tomlin 1994)
- 21000 (21°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
- 11.3 \times 10^{-4} (20°C, Wolfiedietrich 1965; Melnikov 1971; Khan 1980)
- 3.73 \times 10^{-4} (20°C, vaporization rate-gravimetric method, Gückel et al. 1973)
11.0 × 10⁻⁴ (Worthing 1979; Hartley & Kidd 1987)
8.90 × 10⁻⁴ (20°C, GC, Seiber et al. 1981)
3.87 × 10⁻⁴ (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temperatures, Kim et al. 1984)
85.0 × 10⁻⁴ (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
41.0 × 10⁻⁴ (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
2.90 × 10⁻⁴ (20°C, Worthing & Hance 1991)
33.3 × 10⁻⁴ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.75 × 10⁻⁴ (20°C, Montgomery 1993)
11.0 × 10⁻⁴ (Tomlin 1994)
0.0363 (gradient GC method; Tsuzuki 2000)
0.0363; 0.11, 0.083 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
6.23 × 10⁻⁶ (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
1.10 × 10⁻⁴ (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
2.66 × 10⁻⁶ (20–21°C, calculated-P/C, Montgomery 1993)
1.15 × 10⁻⁴ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:
-0.29 (Hamaker 1975; Kenaga & Goring 1980)
-0.294 (shake flask-GC, Freed et al. 1979)
0.79 (20 ± 2°C, shake flask-UV, Briggs 1981)
0.70 (22°C, shake flask-GC, Bowman & Sans 1983)
0.50, 0.78 (recommended, Hansch & Leo 1985)
2.71 (Kanazawa 1989)
0.699 (Worthing & Hance 1991; Milne 1995)
0.51–0.78 (Montgomery 1993)
0.50 (recommended, Sangster 1993)
0.704 (Tomlin 1994)
0.78 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.00 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log K<sub>OC</sub>:
1.23 (soils, calculated, Kenaga 1980a; quoted, Howard 1991)
0.72 (20 ± 2°C, shake flask-UV and reported as log K<sub>OM</sub>, Briggs 1981)
1.43 (average of 2 soils, Kanazawa 1989)
1.26, 1.56 (clay loam soil, Kanazawa 1989)
0.716 (clay soil, Kanazawa 1989)
0.72, 1.47 (reported as log K<sub>OM</sub>, estimated as log K<sub>OM</sub>, Magee 1991)
1.20, 1.39 (soil, quoted exp., calculated-χ and fragment contribution, Meylan et al. 1992)
0.132 (estimated-QSAR and SPARC, Kollig 1993)
0.96 (Montgomery 1993)
1.00 (estimated-chemical structure, Lohninger 1994)
1.21; 1.72 (sandy loam soil, sandy loam sand, Tomlin 1994)
1.20 (soil, calculated-MCI 1<sup>1</sup>χ, Sabljic et al. 1995)
1.20; 1.70, 1.85 (soil, quoted exp.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
Insecticides

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

Volatileization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 0.469–4.69$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2} = 0.8$ h at pH 9 and $t_{1/2} = 21$ h at pH 2 both at 70°C (Melnikov 1971; quoted, Freed et al. 1977)

neutral rate constant $k = 1.7 \times 10^{-4}$ h$^{-1}$ with a calculated $t_{1/2} = 118$ h at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Montgomery 1993);

first-order $t_{1/2} = 2822$ h, based on measured neutral and base catalyzed hydrolysis rate constants (Ellington et al. 1987; quoted, Howard et al. 1991);

rate constant $k = 1.68$ yr$^{-1}$ at pH 7.0 and 25°C (Kollig 1993);

$t_{1/2} = 12$ d at pH 9 (Tomlin 1994)

$t_{1/2} = 120$ d at pH 2, $t_{1/2} = 120$ d at pH 7 and $t_{1/2} = 0.0038$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 264–1344$ h, based on river die-away test data (Eichelberger & Lichtenburg 1971; quoted, Howard et al. 1991) and soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1056–5376$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biomechanica:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.469–4.69$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 264–1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}($aerobic$) = 11$ d, $t_{1/2}($anaerobic$) = 44$ d in natural waters (Capel & Larson 1995)

$t_{1/2} = 423$ d at 6°C, 193h at 23°C in darkness for Milli-Q water; $t_{1/2} = 171$ d at 6°C, $t_{1/2} = 43$ d at 22°C in darkness, $t_{1/2} = 29$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 173$ d at 6°C, $t_{1/2} = 29$ d at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2} = 219$ d at 6°C, $t_{1/2} = 36$ d at 22°C in darkness, $t_{1/2} = 74$ d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).

Ground water: $t_{1/2} = 528–2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 264–888$ h, based on soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991);

selected $t_{1/2} = 7.0$ d (Wauchope et al. 1992; Hornsby et al. 1996);

aerobic $t_{1/2} = 2–4.1$ d in soil and photolytic $t_{1/2} = 7–16$ d on soil surface (Tomlin 1994);

$t_{1/2} = 7.0$ d (selected, Halfon et al. 1996).

Biota: disappearance rate and half-life from treated plants: $t_{1/2} = 2.95$ d for cabbage, $t_{1/2} = 3.40$ d for tomato leaves and $t_{1/2} = 2.40$ d for tomato fruits (Othman et al. 1987).
18.1.1.33 Disulfoton

Common Name: Disulfoton
Synonym: Di-Syston, Dimaz, Disipton, Disystox, Dithiosystox, Frumin AL, Glebofos, Solvirex
Chemical Name: \( O,O\)-diethyl \( S\)-\([2-(ethylthio) ethyl] \) phosphorodithioate; phosphorodithioic acid, \( O,O\)-diethyl \( S\)-\([2-(ethylthio)ethyl] \) ester

Uses: insecticide to control aphids, thrips, mealybugs, and other sucking insects, and spider mites in potatoes, vegetables, cereals, maize, sorghum, rice, soybeans, groundnuts, lucerne, clover, sugar cane, sugar beet, hops, strawberries, cotton, coffee, pineapples, tobacco, ornamentals, fruit and nut crops, and forestry nurseries; also used as acaricide.

CAS Registry No: 298-04-4
Molecular Formula: \( \text{C}_8\text{H}_{19}\text{O}_2\text{PS}_3 \)
Molecular Weight: 274.405
Melting Point (°C): 

\(-25\) (Milne 1995; Lide 2003)

Boiling Point (°C):

\(62.0\) (at 0.01 mmHg, Hartley & Kidd 1987)
\(128\) (at 1 mmHg, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm\(^2\) at 20°C):

\(1.144\) (Hartley & Kidd 1987; Tomlin 1994)
\(1.14\) (Worthing & Hance 1991)

Molar Volume (cm\(^3\)/mol):

282.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, \( pK_a \):

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/m\(^3\) or mg/L at 25°C or as indicated):

66 (Günther 1968)
25 (20°C, Melnikov 1971; Spencer 1973)
25 (Martin & Worthing 1977)
16.3 (19.5°C, shake flask-GC, Bowman & Sans 1979, 1983b)
25 (22°C, Khan 1980; Worthing & Walker 1983)
25 (22°C, Hartley & Kidd 1987)
12 (22°C, Worthing & Hance 1991)
12 (20°C, Tomlin 1994)
12 (22°C, Milne 1995)
29.9, 29.9 (supercooled liquid \( S_L \); literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated):

0.024 (20°C, vapor density, MacDougall & Archer 1964)
\( \log (P/\text{mmHg}) = 10.20 – 4084.80/(T/K) \); temp range 10–40°C (vapor density, MacDougall & Archer 1964)
0.024 (20°C, Eichler 1965)
0.024 (20°C, Melnikov 1971; Khan 1980)
0.024 (Worthing 1983)
0.0041 (20°C, GC-Rt correlation, Kim et al. 1984; Kim 1985)
0.024 (20°C, Hartley & Kidd 1987)
0.020 (20°C, selected, Suntio et al. 1988)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated)</td>
<td>0.22 (20°C, calculated-P/C, Suntio et al. 1988)</td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log $K_{OW}$</td>
<td>3.04 (Callahan et al. 1979)</td>
</tr>
<tr>
<td>Octanol/Air Partition Coefficient, log $K_{OA}$</td>
<td>8.39 (final adjusted value FAV, Muir et al. 2004)</td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF</td>
<td>2.00 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)</td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log $K_{OC}$</td>
<td>3.25 (soil, Hamaker &amp; Thompson 1972; Kenaga 1980; Kenaga &amp; Goring 1980)</td>
</tr>
</tbody>
</table>

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

Volatile: gas exchange $t_{1/2} = 900$ d for winter and $t_{1/2} = 360$ d for summer in Rhine River (Wanner et al. 1989).

Photolysis: photolytic $t_{1/2} = 1000$ d for winter and $t_{1/2} = 100$ d for summer in the Rhine River (Wanner et al. 1989); $t_{1/2} = 1–4$ d (Tomlin 1994)

Apparent first-order rate constant phototransformation at $\lambda > 285$ nm, $k = (1.38 \pm 0.12) \times 10^{-2}$ h$^{-1}$ in puriﬁed water, and $k = (1.68 \pm 0.12) \times 10^{-2}$ h$^{-1}$ in Capot river water with $t_{1/2} \sim 40$ h (Zamy et al. 2004)

Oxidation: half-life ranged from $t_{1/2} \sim 5$ h of midday sunlight during summer to $t_{1/2} = 12$ h during winter estimated from kinetic data for oxygenation reactions photosensitized by humic substances in water exposed to sunlight (Zepp et al. 1981);

photooxidation $t_{1/2} = 0.50–4.80$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2} = 103$ d, based on measured overall rate constant $k = 2.8 \times 10^{-4}$ h$^{-1}$ at pH 7, 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991);

abiotic hydrolysis $k = 1.3 \times 10^{-7}$ s$^{-1}$ under neutral condition, $k = 2.0 \times 10^{-3}$ s$^{-1}$ under base-catalyzed condition at 20°C and hydrolysis $t_{1/2} = 170$ d at 11°C, pH 9 and $t_{1/2} = 62$ d in summer were predicted in Rhine River (Wanner et al. 1989);

$t_{1/2} = 3.04$ yr in water at pH 1–5 and at 20°C; 1.2 d at pH 7 and $t_{1/2} = 7.2$ h at pH 9 both at 70°C (Worthing & Hance 1991);

rate constant $k = 3.23$ yr$^{-1}$ at pH 7.0 and 25°C (Kollig 1993);

$t_{1/2} = 133$ d at pH 4, $t_{1/2} = 169$ d at pH 7, and $t_{1/2} = 131$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{1/2} < 14$ d, rapidly oxidized in soil (Szeto et al. 1983)

primary biodegradation rate constant $k = 0.2$ µg$^2$ L$^2$ d$^{-1}$ with $t_{1/2} = 41$ d, and the degradation $t_{1/2} = 7–41$ d for winter and $t_{1/2} = 4–28$ d for summer in Rhine River (Wanner et al. 1989);

aqueous aerobic $t_{1/2} = 72–504$ h, based on aerobic soil field data and reported half-lives for soil (Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 288–2016$ 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: $t_{1/2} = 0.50–4.80$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: gas exchange $t_{1/2} = 900$ d for winter, $t_{1/2} = 360$ d for summer; abiotic hydrolysis half-lives of 170 d for winter, 62 d for summer; photolytic transformation $t_{1/2} = 1000$ d for winter, $t_{1/2} = 200$ d for summer and primary biodegradation $t_{1/2} = 7–41$ d for winter, $t_{1/2} = 8–28$ d for summer in Rhine River under environmental conditions (Wanner et al. 1989);

overall $t_{1/2} = 72–504$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

$40$ h upon photolysis in Capot river water (Zamy et al. 2004)

Ground water: $t_{1/2} = 144–1008$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated persistence of 4 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982);

$72–504$ h, based on aerobic soil field data (Szeto et al. 1983; quoted, Howard et al. 1991) and reported half-lives for soil (Domsch 1984; quoted, Howard et al. 1991);

$5$ d from screening model calculations (Jury et al. 1987b);

estimated $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{1/2} = 9$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2} = 5$ d from screening model calculations (Jury et al. 1987b).
18.1.1.34 Endosulfan

Common Name: Endosulfan
Synonym: Benzoepin, Beosit, Bio 5462, Chlorthiepin, Crissulfan, Cyclodan, Endocel, ENT 23979, FMC 5462, Hildan, Hoe 2671, Insectophene, KOP-thiodan, Malix, NCI-C00566, Niagara 5462, OMS-570, Thifor, Thimul, Thiodan, Thionex, Thiosulfan, Tionel, Tiavel

Chemical Name: 1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dimethyl cyclic sulfite; 1,2,3,4,7,7-hexachlorobicyclo-2,2,1-hepten-5,6-bisoxymethylene sulfite; (1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-en-2,3-ylene-bismethylene)-sulfite; 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepine 3-oxide

Uses: insecticide for vegetable crops and also used as acaricide.

CAS Registry No: 115-29-7; 959-98-8 (α-endosulfan, endosulfan I); 33213-65-9 (β-endosulfan, endosulfan II)

Molecular Formula: C₉H₆Cl₆O₃S

Molecular Weight: 406.925

Melting Point (°C):
- 70–100 (tech. grade, Worthing & Hance 1991; Milne 1995)
- 70–100, 108–110 (α-endosulfan, β-endosulfan, Suntio et al. 1988)
- 106, 207–209 (α-endosulfan, β-endosulfan, Montgomery 1993)
- 109.2, 213.3 (α-endosulfan, β-endosulfan, Tomlin 1994)
- 106, 109.2 (Milne 1995)

Boiling Point (°C):
- 106 (at 0.7 mmHg, Hartley & Kidd 1987; Milne 1995)

Density (g/cm³ at 20°C):
- 1.80 (tech. grade, Tomlin 1994)
- 1.745 (Milne 1995; Montgomery 1993)

Molar Volume (cm³/mol):
- 312.8 (calculated-Le Bas method at normal boiling point,)

Dissociation Constant, pKₐ:

Enthalpy of Fusion, ∆H₅₀ (kJ/mol):

Entropy of Fusion, ∆S₅₀ (J/mol K):

Fugacity Ratio at 25°C (assuming ∆S₅₀ = 56 J/mol K), F:
- 0.22. 0.13 (20°C, α-, β-endosulfan, Suntio et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C pr as indicated):
- 0.53 (α-endosulfan, generator column-GC, Weil et al. 1974)
- 0.286 (β-endosulfan, generator column-GC, Weil et al. 1974)
- <1.0 (Wauchope 1978)
- 0.050 (Weber et al. 1980)
- 0.510 (α-endosulfan, 20°C, shake flask-GC, Bowman & Sans 1983a)
- 0.45 (β-endosulfan, 20°C, shake flask-GC, Bowman & Sans 1983a)
- 0.06–0.15 (U.S. EPA 1984; McLean et al. 1988)
- 0.32 (22°C, Hartley & Kidd 1987)
- 0.15 (20°C, selected, Suntio et al. 1988)
- 0.32 (α-endosulfan at 22°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 0.33 (β-endosulfan at 22°C, Worthing & Hance 1991; Tomlin 1994)
- 0.32 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.53 (α-endosulfan, Montgomery 1993)
- 0.28 (β-endosulfan, Montgomery 1993)
3.75, 3.63 (α-endosulfan, supercooled liquid $S_L$: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
1.71, 2.56 (α-endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
32.1, 36.2 (β-endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):

0.00133 (Martens 1972; Khan 1980)
0.013 (endosulfan I, Barlow 1978)
> 0.00013 (20–25°C, Weber et al. 1980)
1.20 (80°C, Hartley & Kidd 1987)
0.0061 (endosulfan I, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
0.0032 (endosulfan II, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
0.0011 (20°C, selected, Suntio et al. 1988)
1.20 (tech. grade at 80°C, Worthing & Hance 1991)
2.27 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00133 (Montgomery 1993)
8.3 × 10⁻⁵ (20°C, 2 to 1 mixture of α- and β-endosulfan, Tomlin 1994)
2.3 × 10⁻⁵ (selected, Halfon et al. 1996)
0.0061, 0.0063 (α-endosulfan, supercooled liquid $P_L$: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
0.0060, 0.0044 (α-endosulfan, supercooled liquid $P_L$: LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
0.0043, 0.0040 (β-endosulfan, supercooled liquid $P_L$: LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

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

1.09 (calculated-P/C, Mabey et al. 1982)
2.98 (20°C, calculated-P/C, Suntio et al. 1988)
0.679, 0.0627 (endosulfan I, II, calculated, Cotham & Bidleman 1989)
1.35 (calculated-P/C an average of α- and β-endosulfan, Howard 1991)
10.23 (α-endosulfan, Montgomery 1993)
1.935 (β-endosulfan, calculated-P/C, Montgomery 1993)
6.45, 13.23 (20°C, tech. grade: distilled water, salt water 33.3l%, wetted wall column-GC, Rice et al. 1997a, b)
6.63, 0.788 (20°C, endosulfan I, II, distilled water, wetted wall column-GC, Rice et al. 1997a, b)
log $K_{AW} = –876.14/(T/K) + 0.4463$; temp range: 8.3–38.2°C, (endosulfan I, distilled water, wetted-wall column-GC, Rice et al. 1997a)
12.89, 2.12 (20°C, endosulfan I, II, salt water 33.3l%, wetted wall column-GC, Rice et al. 1997a, b)
8.65, 8.48; 9.31 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 171% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
8.77, 8.04; 9.12 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 161% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
7.14, 9.21; 8.43 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 121%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
0.719, 0.040 (α- β-endosulfan, wetted wall column-GC, Altschuh et al. 1999)
6.99 (20°C, Endosulfan I, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log $K_{AW} = 0.446 – 876/(T/K)$, (Endosulfan I, van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
0.715, 0.699 (α-endosulfan, literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
0.72, 0.70 (α-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
0.040, 0.045 (β-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.55, 3.62 (α-, β-endosulfan, Ali 1978)
3.83 (α-endosulfan, shake flask-GC, Hermens & Leeuwangh 1982)
3.83 (α-endosulfan, Hansch & Leo 1985)
4.74, 4.78 (α-, β-endosulfan, calculated-fragment const., Noegrohoati & Hammers 1992)
3.55, 3.62 (α-, β-endosulfan, Montgomery 1993)
4.74, 4.79 (α-, β-endosulfan at pH 5, Tomlin 1994)
3.62, 3.83 (α-, β-endosulfan, Hansch et al. 1995)
3.84 (Pomona-database, Müller & Kördel 1996)
5.09 (α-endosulfan, literature-derived value LDV, Muir et al. 2004)
4.74, 4.94 (α-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
4.78, 4.78 (β-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:


$\log K_{OA} = -5.90 + 4333/(T/K)$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
8.64 (α-endosulfan, final adjusted value FAV, Muir et al. 2004)
8.63, 8.49 (α-endosulfan, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

–3.66 (beef biotransfer factor log $B_b$, correlated-$K_{OW}$, Beck et al. 1966)
2.78 (α-endosulfan for mussel, Ernst 1977;)
–1.52, –1.22 (α-, β-endosulfan, bioaccumulation factor log BF, adipose tissue in female Albino rats, Dorough et al. 1978)
2.63, 2.44 (α-, β-endosulfan, paddy field fish, Soon & Hock 1987)
1.91, 2.33 (α-, β-endosulfan, paddy field fish, Tejada 1995)
3.55; 3.65 (α-endosulfan for Oncorhynchus mykiss, wet wt. basis; quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

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

3.46 (α-endosulfan, estimated, Lyman et al. 1982; quoted, Howard 1991)
3.83 (β-endosulfan, calculated-S, Lyman et al. 1982; quoted, Howard 1991)
4.00 (α- or β-endosulfan, estimated-QSAR & SPARC, Kollig 1993)
3.31, 3.37 (α-endosulfan, β-endosulfan, calculated, Montgomery 1993)
4.09 (soil, α-endosulfan, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
4.09 (estimated-chemical structure, Lohninger 1994)
3.48–4.30 (Tomlin 1994)
4.09 (α-endosulfan, HPLC-screening method, Kördel et al. 1995)
4.09; 5.24 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.90 (soil, estimated-general model, Gramatica et al. 2000)

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

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2} = 2.5–24.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air with a deoxygenated endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: first-order $t_{1/2} = 218$ h, based on neutral aqueous hydrolysis rate constant $k = (3.2 \pm 2.0) \times 10^{-3}$ h$^{-1}$ for α-Endosulfan at pH 7 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);
first-order $t_{1/2} = 187$ h, based on neutral aqueous hydrolysis rate constant $k = (3.7 \pm 2.0) \times 10^{-3}$ h$^{-1}$ for β-endosulfan at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);
rate constant \( k = 6.1 \times 10^{-2} \text{ yr}^{-1} \) for \( \alpha \)-endosulfan at pH 7 and 25°C and rate constant \( k = 8.9 \times 10^{-2} \text{ yr}^{-1} \) for \( \beta \)-endosulfan at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic \( t_{1/2} = 48–336 \text{ h} \), based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Bowman et al. 1965; quoted, Howard et al. 1991);

first-order rate constants \( k = -0.00502 \text{ h}^{-1} \) in nonsterile sediment, \( k = -0.00796 \text{ h}^{-1} \) in sterile sediment by shake-tests at Range Point, first-order \( k = -0.0157 \text{ h}^{-1} \) in nonsterile water, and \( k = -0.0325 \text{ h}^{-1} \) in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants \( k = -0.00165 \) to \( -0.00296 \text{ h}^{-1} \) in nonsterile sediment, \( k = -0.00426, -0.00545 \text{ h}^{-1} \) in sterile sediment by shake-tests at Davis Bayou and first-order rate constants \( k = -0.00335 \) to \( -0.00490 \text{ h}^{-1} \) in nonsterile water and \( k = -0.0130, -0.00866 \text{ h}^{-1} \) in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

\( t_{1/2} \) (aerobic) = 2 d, \( t_{1/2} \) (anaerobic) = 8 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\( k_1 = 12.3 \text{ h}^{-1}; k_2 = 0.0205 \text{ h}^{-1} \) (mussel from \( \alpha \)-endosulfan, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

**Air:** \( t_{1/2} = 2.5–24.8 \text{ h} \), based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air with a deoxygenated Endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991);

\( t_{1/2} = 9.2 \pm 4 \text{ yr} \) at Eagle Harbor in the Great Lake’s atmosphere. (Buehler et al. 2004).

**Surface water:** persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971);

\( t_{1/2} = 50 \text{ d} \) for \( \alpha \)- and \( \beta \)-endosulfan respectively for surface waters in case of first order reduction process may be assumed and estimated \( t_{1/2} \sim 30–300 \text{ d} \) for \( \beta \)-endosulfan in lakes in the Netherlands (Zoeteman et al. 1980);

\( t_{1/2} = 4.5–218 \text{ h} \), based on aqueous hydrolysis half-lives for both \( \alpha \)- and \( \beta \)-endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991)

\( t_{1/2} = 1.3 \text{ d} \) in rice paddy water (Tejada et al. 1993; quoted, Abdullah et al. 1997)

\( t_{1/2} \) (aerobic) = 2 d, \( t_{1/2} \) (anaerobic) = 8 d, hydrolysis \( t_{1/2} = 360 \text{ d} \) at pH 2, \( t_{1/2} = 9.1 \text{ d} \) at pH 7 and \( t_{1/2} = 0.00029 \text{ d} \) at pH 12 in natural waters (Capel & Larson 1995)

**Ground water:** estimated \( t_{1/2} = 30–300 \text{ d} \) in lakes and Ground water (\( \beta \)-Endosulfan, Zoeteman et al. 1980);

\( t_{1/2} = 4.5–218 \text{ h} \), based on aqueous hydrolysis half-lives for both \( \alpha \)- and \( \beta \)-endosulfan at pH 7 and 9 and 25°C respectively (Ellington et al. 1987; quoted, Howard et al. 1991).

**Sediment:**

\( t_{1/2} = 4.5–218 \text{ h} \), based on aqueous hydrolysis half-lives for both \( \alpha \)- and \( \beta \)-endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991);

\( t_{1/2} > 50 \text{ d} \) and subject to plant uptake via volatilization (Ryan et al. 1988);

selected \( t_{1/2} = 50 \text{ d} \) (Wauchope et al. 1992; Hornsby et al. 1996);

\( t_{1/2} = 1.2 \text{ d} \) in rice soil (Tejada et al. 1993; quoted, Abdullah et al. 1997);

soil \( t_{1/2} = 120 \text{ d} \) (Paik et al. 1992);

degraded in soil with \( t_{1/2} = 30–70 \text{ d} \) (Tomlin 1994); 50 d (selected, Halfon et al. 1996)

\( t_{1/2} = 5–7 \text{ yr} \) in soil (Geyer et al. 2000)

**Biota:** \( t_{1/2} = 33.8 \text{ h} \) in mussels (\( \alpha \)-endosulfan, Ernst 1977);

\( t_{1/2} = 1.0 \text{ d} \) in rice leaves (Tejada et al. 1993; quoted, Abdullah et al. 1997).
TABLE 18.1.1.34.1
Reported octanol-air partition coefficients of α-endosulfan at various temperatures

Shoeib & Harner 2002

generator column-GC/MS

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>9.7188</td>
</tr>
<tr>
<td>10</td>
<td>9.3591</td>
</tr>
<tr>
<td>15</td>
<td>9.1651</td>
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<tr>
<td>20</td>
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<tr>
<td>25</td>
<td>8.6772</td>
</tr>
<tr>
<td>25</td>
<td>8.638</td>
</tr>
</tbody>
</table>

log K_{OA} = A + B/(T/K)
A = -5.902
B = 4333

enthalpy of phase change
ΔH_{OA}(kJ mol^{-1}) = 83.0

FIGURE 18.1.1.34.1 Logarithm of K_{OA} versus reciprocal temperature for α-endosulfan.
18.1.1.35 Endrin

Common Name: Endrin
Synonym: Endrex, ENT 17521, Hexadrin, Isodrin epoxidek, Mendrin, NA 2761, NCI-C00157, Nendrin, RCRA
Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4-exo-5,8-dimethano-naphthalene
Uses: Insecticide/Avicide/Rodenticide
CAS Registry No: 72-20-8
Molecular Formula: C12H8Cl6O
Molecular Weight: 380.909

Melting Point (°C):
- 245 (dec, Lide 2003)

Boiling Point (°C):
- 245 (dec. Montgomery 1993)

Density (g/cm³ at 20°C):
- 1.70, 1.65 (pure, technical, at 25°C, Montgomery 1993)

Molar Volume (cm³/mol):
- 318.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
- 23.88 (Ruelle & Kesselring 1997)

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

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.00694 (mp at 245°C)

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):
- 0.23* (shake flask-UV, measured range 25–45°C, Richardson & Miller 1960)
- 0.26 (rm. temp., shake flask-GC, Robeck et al. 1965)
- 0.23 (Günther et al. 1968)
- 0.25* (shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
- 0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 and 5.0µ, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
- 0.26 (generator column-GC/ECD, Weil et al. 1974)
- 0.10 (Weber et al. 1980)
- 0.024 (Bruggeman et al. 1981)
- 0.25 (misquoted as 0.25 µg/L from Biggar & Riggs, Howard 1991)
- 0.22–0.26 (Montgomery 1993)
- 0.23 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 0.105, 0.000065 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- 1.03, 1.14 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

\[
\log [C_\text{L}(\text{mol m}^{-3})] = -1022/(T/K) + 0.86 \quad \text{(supercooled liquid, linear regression of literature data, Shen & Wania 2005)}
\]

Vapor Pressure (Pa at 25°C or as indicated):
- \(4.00 \times 10^{-4}\) (20°C, Bowery 1964)
- \(2.67 \times 10^{-5}\) (Eichler 1965; Melnikov 1971; Martin 1972; Quellette & King 1977)
Insecticides

2.67 × 10⁻⁵ (20–25°C, Weber et al. 1980)
1.17 × 10⁻⁵ (20°C, selected exptl. value, Kim 1985)
2.00 × 10⁻⁵ (20°C, selected, Suntio et al. 1988)
9.33 × 10⁻⁵ (25°C, Montgomery 1993)
1.38 × 10⁻³ (20–25°C, supercooled liquid value, Majewski & Capel 1995)
0.0052, 0.0031 (supercooled liquid P L; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.8 × 10⁻⁴ (calculated-P/C, Mabey et al. 1982)
0.042 (Ryan et al. 1988)
0.033 (20°C, calculated-P/C, Suntio et al. 1988)
0.762 (calculated, Howard 1991)
0.0507 (calculated-P/C, Montgomery 1993)
0.644 (wetted wall column-GC, Altschuh et al. 1999)
0.64, 1.1 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K⁰_W:
5.60 (calculated, Neely et al. 1974)
4.56 (RP-HPLC-RT correlation, Veith et al. 1979)
5.34 (Kenaga & Goring 1980)
3.21 (Rao & Davidson 1980)
4.82 (Veith & Kosian 1982)
5.01 (HPLC-RT correlation, Eadsforth 1986)
5.28 (HPLC-RT correlation, Liu & Qian 1988)
5.195 ± 0.005 (slow-stirring method, De Bruijn et al. 1989)
3.21–5.34 (Montgomery 1993)
4.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
5.20 (recommended, Hansch et al. 1995)
4.71 (RP-HPLC-RT correlation, Finizio et al. 1997)
5.20, 4.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K⁰_O at 25°C and reported temperature dependence equation. Additional data
8.13, 8.32 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
2.40–2.18 (bluegills, Bennett & Day 1970)
2.60–2.88 (channel catfish, Argyle et al. 1973)
3.21 (channel catfish, 55-d exposure, Argyle et al. 1973)
3.13, 4.69 (Gambusia, Physa, Metcalf et al. 1973)
3.11, 4.69, 3.66 (fish, snail, algae, Metcalf et al. 1973)
2.83, 2.49, 2.48 (fish, mosquitoes, Daphnia, 3-d expt. with no dietary routes, Metcalf et al. 1973)
3.43 (oyster, Mason & Rowe 1976)
3.28 (mussel, Ernst 1977)
3.24 (calculated-K⁰_W, Mackay 1982)
4.02; 4.18; 3.85 (flagfish, 30-d exposure; 65-d exposure; 110-d exposure, Hermanutz 1978)
3.70 (fathead minnow, Jarvinen & Tyo 1978)
3.17 (mosquito fish, 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
3.66 (fathead minnow, 300-d exposure, Veith et al. 1979; Veith & Kosian 1983)
3.66 (Oedogonium sp., Baughman & Paris 1981)
3.85–4.18 (flag fish, mosquito fish, Veith & Kosian 1983)
3.24, 3.18 (mussel, calculated-$K_{ow}$ & models, Zaroogian et al. 1985)
3.17 (fathead minnow, quoted from Veith et al. 1979, Zaroogian et al. 1985)
3.40 (Isnard & Lambert 1988)
3.13–4.0 (fish, quoted, Howard 1991)
3.85 (fathead minnow, whole body, after 300-d exposure, Howard 1991)
3.21–3.30 (channel catfish, after 41- and 55-d exposure, Howard 1991)
4.18 (flagfish, whole body after 65-d exposure, Howard 1991)
3.52–3.68 (sheepshead minnow, 33-d exposure for embryojuveniles, Howard 1991)
2.70–3.10 (shellfish, Howard 1991)
4.69, 3.22–3.44, 3.48 (snail, oyster, grass shrimp, mussel, Howard 1991)
2.15–2.30 (algae, Howard 1991)
3.83 (fish, reported as log $BAF_w$, LeBlanc 1996)
3.28, 5.28 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.22, 5.14 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.44, 5.37 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.42 (clam: wet wt basis, Geyer et al. 2000)
3.66, 5.18 (fathead minnow, uptake 300-d: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log $K_{oc}$ at 25°C or as indicated:
4.53 (calculated, Kenaga 1980, quoted, Howard 1991)
5.36 (calculated-S, Mill et al. 1980; quoted, Adams 1987)
4.00 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.00; 4.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2} = 9.6$ d from a model river 1-m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{1/2} > 14$ yr from a model pond (Howard 1991).

Photolysis:
Oxidation:
$$k(aq.) = (2.7 \pm 0.7) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$$ for the reaction with OH radical in aqueous solution (Fenton reaction) at 24 ± 1°C and pH 2.8 (Haag & Yao 1992) with reference to $4.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of DPCP with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992);
$$k(aq.) = (1.3 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$$ for the reaction with OH radical in aqueous solution at 24 ± 1°C and pH 3.4 (Haag & Yao 1992) with reference to $8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of lindane with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992).

Oxidation:
$$k(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$$ for direct reaction with ozone in water at pH 2.7–6.4 and 23 ± 3°C, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Hydrolysis: $t_{1/2} = 4$ yr at least (Callahan et al. 1979).

Biodegradation: $t_{1/2} = 5–14$ d in thick anaerobic sewage sludge (Howard 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$$-\log k_2 = 1.99 \text{ h}$$ (oyster, Mason & Rowe 1976; quoted, Hawker & Connell 1986)
$$\log k_1 = 1.5 \text{ h}^{-1}; -\log k_2 = 1.78 \text{ h}$$ (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:
Air: $t_{1/2} = 1.45$ h was predicted for reaction with hydroxyl radical (Howard 1991).
Surface water: $t_{1/2} > 8$ wk in river water (Eichelberger & Lichtenberg 1971);
measured $k_{a1}(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and 23 ± 3°C, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Ground water:
Sediment:
Insecticides

Soil: $t_{1/2} \sim 12$ yr in Congaree sandy loam soil (Nash & Woolson 1967);
field $t_{1/2} = 63$ d for sugar cane in soil (Willis & Hamilton 1973; quoted, Nash 1983);
moderately persistent in soil with $t_{1/2} = 20–100$ d (Willis & McDowell 1982);
microagroecosystem $t_{1/2} = 33$ d in moist fallow soil (Nash 1983);
$t_{1/2} > 50$ d in soil (Ryan et al. 1988);
selected field $t_{1/2} = 4300$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
$t_{1/2} \sim 12$ yr in soil (Geyer et al. 2000)

Biota: elimination $t_{1/2} = 24$ h (Ernst 1977, quoted, Callahan et al. 1979).

TABLE 18.1.1.35.1
Reported aqueous solubilities and octanol-air partition coefficients of endrin at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Richardson &amp; Miller 1960</td>
<td>Biggar &amp; Riggs 1974</td>
</tr>
<tr>
<td></td>
<td>shake flask-UV spec.</td>
<td>shake flask-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
<td>S/g·m$^{-3}$</td>
</tr>
<tr>
<td></td>
<td>particle size 0.01µ</td>
<td>0.05µ</td>
</tr>
<tr>
<td>25</td>
<td>0.23</td>
<td>15</td>
</tr>
<tr>
<td>35</td>
<td>0.38</td>
<td>25</td>
</tr>
<tr>
<td>45</td>
<td>0.51</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
</tr>
</tbody>
</table>

log $K_{OA} = A + B/(T/K)$
A $-11.75$
B $6067$

enthalpy of phase change
$\Delta H_{OA}/(kJ mol^{-1}) = 84.9$

FIGURE 18.1.1.35.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for endrin.
FIGURE 18.1.35.2 Logarithm of $K_{OA}$ versus reciprocal temperature for endrin.
18.1.1.36 Ethiofencarb

Common Name: Ethiofencarb
Synonym: Croneton, Bay-Hox-1901
Chemical Name: α-ethylthio-o-tolyl methylcarbamate
CAS Registry No: 29973-13-5
Uses: insecticide
Molecular Formula: C₁₁H₁₄NO₂S
Molecular Weight: 225.307
Melting Point (°C):
Boiling Point (°C):
decomposes on distillation (Hartley & Kidd 1987, Tomlin 1994)
Density (g/cm³ at 20°C):
1.1473 (Hartley & Kidd 1987, Worthing & Walker 1987; Montgomery 1993)
1.231 (20°C, Tomlin 1994)
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ:
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: 0.827 (mp at 33.4°C)
Water Solubility (g/m³ or mg/L at 25°C):
1820 (20°C, Worthing & Walker 1987)
1800 (20°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C):
6.67 × 10⁻⁴ (Spencer 1982)
0.013 (30°C, Hartley & Kidd 1987; Worthing & Walker 1987)
4.506 × 10⁻⁴ (20°C, Montgomery 1993)
0.00045, 0.00094, 0.026 (20, 25, 50°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol):
5.37 × 10⁻³ (calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log Kₐw:
0.98 (calculated-Montgomery 1993)
2.04 (Tomlin 1994)
4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)
Octanol/Air Partition Coefficient, log Kₐₐ:
Bioconcentration Factor, log BCF or log Kₐ:
Sorption Partition Coefficient, log Kₐₐₐ:
1.84 (calculated, Montgomery 1993)
Environmental Fate Rate Constants or Half-Lives:

Volatileization:
Photolysis: photodegradation in sunlight is very rapid (Tomlin 1994).
Oxidation:
Hydrolysis: hydrolyzed in alkaline solution (Tomlin 1994).
Biodegradation:

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

Half-Lives in the Environment:
Surface water: in isopropanol/water (1:1, 37–40°C) solutions, half-lives were $t_{1/2} = 300$ d at pH 2, $t_{1/2} = 45$ h at pH 7 and $t_{1/2} = 5$ min at pH 11.4 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).
### 18.1.1.37 Ethion

![Chemical Structure](image)

**Common Name:** Ethion  
**Synonym:** AC 3422, Bladan, diethion, Embathion, ENT 24105, Ethanox, Ethiol, Ethodan, Ethopaz, FMC 1240, Fosfono 50, Hylemax, Hylenox, Itopaz, KWIT, NA 2783, NIA 1240, Niagara 1240, Nialate, Vegfru fosmite  
**Chemical Name:** bis(S-dimethoxyphosphiniothioyl)mercapto)methane; \(O,O,O',O'-\text{tetraethyl-}S,S'\)-methylene bis(phosphorodithioate); \(O,O,O',O'-\text{tetraethyl-}S,S'\)-methylene-bisphosphorothiolothionate

**Uses:** nonsystemic insecticide and acaride used on apples.

**CAS Registry No:** 563-12-2  
**Molecular Formula:** \(C_9H_{22}O_4P_2S_4\)  
**Molecular Weight:** 384.476

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
</table>
| Melting Point (°C) | –12 to –15 (Montgomery 1993; Tomlin 1994; Milne 1995)  
–13 (Lide 2003) |
| Boiling Point (°C) | 164–165 (at 0.3 mmHg, Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Milne 1995) |
| Density (g/cm³ at 20°C) | 1.22 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995) |
| Molar Volume (cm³/mol) | 350.2 (calculated-Le Bas method at normal boiling point) |
| Dissociation Constant, \(pK_a\) |  |
| 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) | 2.0 (Metcalf 1971, 1974)  
0.60 (Miles 1976; Miles & Harris 1978)  
1.0 (20–25°C, selected, Willis & McDowell 1982; Gerstl & Helling 1987)  
1.1 (19.5°C, shake flask-GC, Bowman & Sans 1983b)  
0.68, 0.76 (20°C, 30°C, Montgomery 1993)  
2.0 (Tomlin 1994) |
| Vapor Pressure (Pa at 25°C) | 0.0002 (Khan 1980; Merck Index 1983, 1989)  
0.0002 (Worthing 1983, Worthing & Hance 1991)  
0.0002 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)  
1.50 × 10⁻⁴ (20°C, selected, Suntio et al. 1988)  
1.58 × 10⁻⁴ (gradient GC method; quoted lit., Tsuzuki 2000)  
1.58 × 10⁻⁴; 4.17 × 10⁻⁵, 1.58 × 10⁻⁴ (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000) |
| Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated) | 0.0699 (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)  
0.032 (20°C, calculated-P/C, Suntio et al. 1988)  
0.0384 (calculated-P/C, Montgomery 1993) |
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 5.07 (Hansch & Leo 1979)
- 5.073 (shake flask-GC, Bowman & Sans 1983b)
- 5.07 (recommended, Sangster 1993)
- 4.28, 5.07 (Montgomery 1993)
- 5.07 (selected, Hansch et al. 1995)

Bioconcentration Factor, log $BCF$:
- 2.77 (estimated-log $K_{OW}$, Howard 1991)
- 2.77 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:
- 4.19 (average of 4 soils, King & McCarthy 1968)
- 4.19 (soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)
- 3.81, 3.94, 4.0 (organic soil, Beverley sandy loam, Plainsfield sand, Sharom et al. 1980)
- 3.66 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 4.19; 4.28 (reported as log $K_{OM}$, estimated as log $K_{OM}$, Magee 1991)
- 4.06, 4.12 (soil, quoted exptl., calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 3.54–4.34 (Montgomery 1993)
- 4.43 (estimated-chemical structure, Lohninger 1994)
- 4.06 (calculated-MCI $\chi$, Sabljevic et al. 1995)
- 3.70, 3.95 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization: using Henry’s law constant, $t_{1/2} \sim 102$ d from a model river 1-m deep, flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991).
- Photolysis:
- Oxidation: photooxidation $t_{1/2} \sim 6.95$ h for the vapor-phase reaction with hydroxyl radicals in air (Howard 1991).
- Hydrolysis: half-lives in water at 25°C and pHs of 4.5, 5.0, 6.0, 7.0 and 8.0 were 99, 63, 58, 25, and 8.4 wk, respectively (Chapman & Cole 1982; quoted, Montgomery 1993);
  - $t_{1/2}$(exptl) = 20.8 wk was determined in buffered distilled water at 30°C between pH 4 and 7, $t_{1/2} = 8.9$ wk at pH 8 and $t_{1/2} = 1$ d at pH 10 (Dierberg & Pfeuffer 1983; quoted, Howard 1991);
  - $t_{1/2} = 390$ d at pH 9 (Tomlin 1994).
- Biodegradation: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);
  - $t_{1/2} = 24$–26 d in both sterilized and unsterilized Florida canal water over 12 wk observation (Dierberg & Pfeuffer 1983; quoted, Howard 1991).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: $t_{1/2} \sim 6.95$ h for the vapor-phase reaction with hydroxyl radical in air (Howard 1991).
- Surface water: $t_{1/2} = 4$ wk in river water (Eichelberger & Lichtenberg 1971).
- Ground water:
- Sediment:
  - Soil: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);
  - selected field $t_{1/2} = 150$ d (Wauchope et al. 1992; Hornsby et al. 1996);
  - $t_{1/2} = 90$ d in soil (Tomlin 1994).
- Biota:
18.1.1.38 Ethoprop

Common Name: Ethoprop
Synonym: ethoprophos
Chemical Name: O-ethyl S,S-dipropylphosphorodithioate
CAS Registry No: 13194-48-4
Uses: insecticide/nematicide
Molecular Formula: C₈H₁₉O₂PS₂
Molecular Weight: 242.340
Melting Point (°C): liquid
  20  (Montgomery 1993)
Boiling Point (°C):
  86–91/0.2 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
Density (g/cm³ at 20°C):
  1.094  (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ:
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  700  (20°C, Hartley & Kidd 1987; Tomlin 1994)
  750  (Worthing & Walker 1987)
  700  (Montgomery 1993)
  750  (selected, Wauchope et al. 1992; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C):
  0.0465  (26°C, Hartley & Kidd 1987)
  0.0465  (20°C, Montgomery 1993)
  0.0507  (selected, Wauchope et al. 1992; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  0.0161  (calculated-P/C, Montgomery 1993; Majewski & Capel 1995)
Octanol/Water Partition Coefficient, log Kₐw:
  3.59  (21°C, Montgomery 1993; Tomlin 1994)
  3.59  (quoted, Sabljic et al. 1995)
Octanol/Air Partition Coefficient, log Kₐₐ:
Bioconcentration Factor, log BCF or log Kₐ:
Sorption Partition Coefficient, log Kₐₑ:
  1.41–2.20  (soil, quoted values, Wauchope et al. 1992)
  1.85  (soil, Wauchope et al. 1992; Hornsby et al. 1996)
  1.82–2.27  (Montgomery 1993)
  1.80  (soil, calculated-MCI, Sabljic et al. 1995)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Hydrolysis: stable in water up to 100°C at pH 7, but rapidly hydrolyzed at 25°C at pH 7 (Worthing 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \approx 87$ d in humus-containing soil at pH 4.5 and $t_{1/2} = 14–28$ d in sandy loam at pH 7.2–7.3 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);

field $t_{1/2} = 87$ d in organic soil, $t_{1/2} = 1–28$ d in sandy soil; others $t_{1/2} = 3–63$ d; recommended $t_{1/2} = 25$ d (Wauchope et al. 1992; Hornsby et al. 1996).
18.1.1.39 Fenitrothion

Common Name: Fenitrothion
Synonym: Accothion, Agria 1050, Agrothion, Arbogal, Cyfen, Cytel, Dybar, Falithion, Fenitox, Kotion, Sumithion
Chemical Name: \(\text{O,O-diethyl } \text{O-4-nitro-m-tolyl phosphorothioate; phosphorothioic acid } \text{O,O-diethyl } \text{O-4-nitro-m-tolyl ester; O,O-diethyl } \text{O-(3-methyl-4-nitrophenyl) phosphorothioate}\)
Uses: insecticide to control boring, chewing and sucking insects in cereals, cotton, maize, sorghum, citrus fruit, pome fruit, stone fruit, soft fruit, vines, bananas, olives, rice, soybeans, beet, sugar cane, oilseed rape, vegetables, lucerne, coffee, cocoa, tea, tobacco, ornamentals and forestry; also used as a public health insecticide to control household insects, flies in animal houses, mosquito larvae, and locusts.
CAS Registry No: 122-14-5
Molecular Formula: \(\text{C}_9\text{H}_{12}\text{NO}_5\text{PS}\)
Molecular Weight: 277.234
Melting Point (°C):
3.4 (Tomlin 1994)
Boiling Point (°C):
164 (at 1 mmHg, Worthing & Hance 1991; Milne 1995)
140–145 (at 0.1 mmHg, dec., Tomlin 1994)
Density (g/cm³ at 20°C):
1.328 (Worthing & Hance 1991; Tomlin 1994)
1.3227 (25°C, Milne 1995)
Molar Volume (cm³/mol):
229.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
7.20 (Kortum et al. 1961; Wolfe 1980)
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):
30 (Macy 1948; Hamaker 1975; Kenaga 1980; Kenaga & Goring 1980)
30 (20°C, Bright et al. 1950; Melnikov 1971; Hamaker 1975)
25.2 (20°C, shake flask-GC, Bowman & Sans 1979)
38.7 (20–25°C, shake flask-GC, Kanazawa 1981)
30 (21°C, Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
8.0 × 10⁻³ (20°C, Melnikov 1971)
7.2 × 10⁻³ (20°C, Freed et al. 1979)
8.0 × 10⁻⁴ (20°C, Hartley & Graham-Bryce 1980; Khan 1980)
5.5 × 10⁻³ (gas saturation method, Addison 1981)
5.4 × 10⁻³ (gas saturation-extrapolated, Addison 1981)
8.0 × 10⁻³ (Budavari 1989)
1.1 × 10⁻² (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
1.5 × 10⁻⁴ (20°C, Worthing & Hance 1991)
0.0180 (20°C, Tomlin 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):

- 0.0942, 0.0669 (exptl., estimated Metcalf et al. 1980)
- 0.0962 (calculated-bond contribution method, Meylan & Howard 1991)
- 0.0012 (calculated-P/C, this work)

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

- 3.38 (20°C, shake flask-GC, Chiou et al. 1977)
- 3.30 (shake flask, Mundy et al. 1978)
- 3.38 (shake flask-GC, Freed et al. 1979)
- 3.36 (Rao & Davidson 1980)
- 3.397 (shake flask-GC, Bowman & Sans 1983b)
- 3.16 (shake flask-HPLC, Moody et al. 1987)
- 3.466 ± 0.003 (shake flask/slow-stirring method, De Bruijn & Hermens 1991; De Bruijn et al. 1993)
- 2.96 (RP-HPLC-RT correlation, Saito et al. 1993)
- 3.03 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 3.30 (recommended, Sangster 1993)
- 3.43 (Milne 1995)
- 3.30 (selected, Hansch et al. 1995)
- 3.03 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.00 (fish in static water, Leo et al. 1971; Kenaga & Goring 1980)
- 2.23 (motsugo, Kanazawa 1975)
- 2.34 (rainbow trout, Takimoto & Miyamoto 1976)
- 2.02 (mussel, McLeese et al. 1979)
- 1.96 (calculated-S, Kenaga 1980)
- 2.39 ($Pseudorasbora parva$, Kanazawa 1981)
- 2.34, 2.17 (mussel, calculated-$K_{ow}$ & models, Zaroogian et al. 1985)
- 2.11 (mussel, Zaroogian et al. 1985)
- 2.74, 2.75 ($Oryzias latipes$, Takimoto et al. 1984)
- 2.48 ($Oryzias latipes$, Takimoto et al. 1987)
- 2.60 (willow shiner, Tsuda et al. 1989)
- 3.36 ± 0.04 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
- 2.37, 2.72 (killifish, De Bruijn & Hermens 1991)
- 2.18, 2.31, 1.48 (minnow, motsugo, mullet, De Bruijn & Hermens 1991)
- 3.54 ($Poecilia reticulata$, De Bruijn & Hermens 1991)
- 2.30, 2.39 (rainbow trout, topmouth gudgeon, De Bruijn & Hermens 1991)
- 1.65, 1.68 ($Oryzias latipes$, Tsuda et al. 1995)

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

- 2.83 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 2.63 (average of 2 soils, Kanazawa 1989)
- 2.54, 2.76 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

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

Volatilization: $t_{1/2} = 6.3$ d from the bottom of Palfrey Lake and $t_{1/2} = 7.2$ d from the surface of Palfrey Lake vs. a calculated $t_{1/2} = 20.6$ d; 0.9 d from Palfrey Brook vs. a calculated $t_{1/2} = 5.40$ d (Metcalf et al. 1980).
Photolysis: disappearance rate constant $k = 0.053 \text{ h}^{-1}$ with calculated first-order $t_{1/2} = 13 \text{ h}$ (Lacorte & Barcelo 1994).

Oxidation:
Hydrolysis: second-order alkaline hydrolysis rate constant $k = 4.2 \times 10^{-3} \text{ M}^{-1} \text{s}^{-1}$ at 27°C (Maquire & Hale 1980; quoted, Wolfe 1980); estimated half-lives at 22°C: $t_{1/2} = 108.8 \text{ d}$ at pH 4, $t_{1/2} = 84.3 \text{ d}$ at pH 7, and $t_{1/2} = 75 \text{ d}$ at pH 9 (Tomlin 1994).
Biodegradation: aerobic degradation $k = 2.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 13.0 \text{ d}$ for control system, $k = 0.4 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 73.0 \text{ d}$ for metabolism, $k = 5.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 8.50 \text{ d}$ for co-metabolism; anaerobic degradation $k = 1.7 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 17.0 \text{ d}$ for control system, $k = 3.9 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 9.6 \text{ d}$ for metabolism, $k = 38.0 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 88 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)
$k_2 = 0.4 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)
$k_1 = 0.070 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)
$k_2 = (3.89 \pm 1.39) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)
$k_1 = (1.13 \pm 0.07) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)
$k_2 = 1.01 \text{ d}^{-1}$ (guppy, calculated-KOW, De Bruijn & Hermens 1991)
$k_2 = (0.28 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)
$k_2 = (0.15 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} = 15–168 \text{ h}$ in summer, Palfrey Lake, Canada at pH 6.7, 11°C under sunlight conditions (Metcalf et al. 1980);
$t_{1/2} = 36–48 \text{ h}$ at pH 7.0–7.5, 19–23°C under sunlight conditions, $t_{1/2} = 518–1188 \text{ h}$ at pH 7.5, 23°C under dark conditions in Lac Bourgeois, Quebec (Greenhalgh et al. 1980);
$t_{1/2} = 5.5 \text{ d}$ and $1.0 \text{ d}$ under aerobic and anaerobic co-metabolism conditions, $t_{1/2} = 73 \text{ d}$ under aerobic metabolism condition (Liu et al. 1981)
$t_{1/2} = 13 \text{ h}$ in winter, irrigation ditch from Ebre Delta, Spain under sunlight conditions, at pH 7.8, 11°C (Lacorte & Barcelo 1994);
$t_{1/2} = 202 \text{ d}$ at 6°C, $t_{1/2} = 62 \text{ d}$ at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 103 \text{ d}$ at 6°C, $t_{1/2} = 31 \text{ d}$ at 22°C in darkness, $t_{1/2} = 4 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 143 \text{ d}$ at 6°C, $t_{1/2} = 27 \text{ d}$ at 22°C in darkness for filtered water at pH 7.3; $t_{1/2} = 224 \text{ d}$ at 6°C, $t_{1/2} = 34 \text{ d}$ at 22°C in darkness, $t_{1/2} = 3 \text{ d}$ under sunlight conditions in seawater (Arcachon Bay, France) at pH 8.1, 22–25°C (Lartiges & Garriques 1995);
$t_{1/2} = 11–19.3 \text{ h}$ at pH 7.8–8.2, 25–20°C under sunlight conditions in rice crop field; $t_{1/2} = 70–74 \text{ h}$ at pH 8.2, 15–18°C under dark conditions from Ebre Delta, Spain (Oubina et al. 1996).

Ground water:

Soil: selected field $t_{1/2} = 4 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{1/2} = 12–28 \text{ d}$ under upland conditions and $t_{1/2} = 4–20 \text{ d}$ under submerged conditions (Tomlin 1994).

Biota: excretion $t_{1/2} = 9.9 \text{ h}$ (willow shiner, Tsuda et al. 1989);
elimination rate constants $k = (0.28 \pm 0.02) \times 10^3 \text{ (NADPH) min}^{-1} \text{mg protein}^{-1}$ and $0.15 \pm 0.02 \times 10^3 \text{ (GSH) min}^{-1} \text{mg protein}^{-1}$ (rainbow trout, De Bruijn & Hermens 1993);
degradation $t_{1/2} = 4 \text{ d}$ in balsam fir and spruce foliage (Tomlin 1994).
18.1.1.40 Fenoxycarb

Common Name: Fenoxycarb
Synonym: Insegar, Logic, Pictyl, Torus, Varikil
Chemical Name: ethyl 2-(4-phenoxyphenoxy)ethylcarbamate; ethyl[2-((p-phenoxy)ethyl]- carbamate
Uses: insecticide to control lepidoptera, scale insects, and psyllids on fruit, cotton and ornamentals; and also cockroaches, fleas, mosquito larvae, and fire ants in public health situations.

CAS Registry No: 79127-80-3
Molecular Formula: C17H19NO4
Molecular Weight: 301.338
Melting Point (°C): 53 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.23 (Tomlin 1994)
Molar Volume (cm³/mol):
344.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH₂₀ (kJ/mol):
Entropy of Fusion, ΔS₂₀ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₂₀ = 56 J/mol K), F: 0.531 (mp at 53°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
6.0 (20°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
5.7 (Worthing & Hance 1991)
6.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
1.7 × 10⁻⁶ (Hartley & Kidd 1987)
7.8 × 10⁻⁶ (20°C, Worthing & Hance 1991)
8.7 × 10⁻⁷ (Tomlin 1994)
1.7 × 10⁻⁶ (20–25°C, selected, Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol):
8.5 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log Kₐq:
4.30 (Worthing & Hance 1991; Milne 1995)
4.07 (Tomlin 1994)
4.30 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.35 (calculated-S as per Kenaga 1980, this work)
3.11 (calculated-Kq as per Kenaga 1980, this work)

Sorption Partition Coefficient, log Kₐq:
3.00 (20–25°C, estimated, Hornsby et al. 1996)

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

Half-Lives in the Environment:
Soil: t½ = 1.7–2.5 months in laboratory soil and water and t½ = few days to 31 d in field soil and water (Tomlin 1994); field t½ = 1 d (20–25°C, selected, Hornsby et al. 1996).
18.1.1.41 Fenpropathrin

Common Name: Fenpropathrin
Synonym: Rody, Danitol, Meothrin, S-3206, Ortho Danitol, Herald, Meothrin
Chemical Name: \((R,S)\)-\(\alpha\)-cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate
CAS Registry No: 64257-84-7 (racemate); 39515-41-8 (unstated stereochemistry)
Uses: insecticide/acaricide (pyrethroid)
Molecular Formula: \(C_{22}H_{23}NO_3\)
Molecular Weight: 349.423
Melting Point (°C):
47 (Lide 2003)
Boiling Point (°C):
1.15 (Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm\(^3\) at 20°C):
1.15 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm\(^3\)/mol):
Dissociation Constant, \(pK_a\): 
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: 0.608 (mp at 47°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C):
0.33 (Hartley & Kidd 1987)
0.0141 (Tomlin 1994)
0.33 (selected, Augustijn-Beckers et al. 1994)
Vapor Pressure (Pa at 25°C):
0.00073 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.00130, 0.00133 (quoted, Augustijn-Beckers et al. 1994)
7.33 × 10\(^{-4}\) (selected, Augustijn-Beckers et al. 1994)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
Octanol/Water Partition Coefficient, \(\log K_{\text{OW}}\):
6.0 (20°C, Tomlin 1994)
Octanol/Air Partition Coefficient, \(\log K_{\text{OA}}\):
Bioconcentration Factor, \(\log BCF\) or \(\log K_{\text{B}}\):
Sorption Partition Coefficient, \(\log K_{\text{OC}}\):
6.75, 3.70 (quoted, estimated, Augustijn-Beckers et al. 1994)
3.70 (soil, estimated and selected, Augustijn-Beckers et al. 1994)
Environmental Fate Rate Constants, \(k\), or Half-Lives:
Volatilization:
Photolysis: degraded principally by photolysis, \(t_{\text{1/2}} = 2.7\) wk in river water (Hartley & Kidd 1987; Tomlin 1994).
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: degraded principally by photolysis, \( t_{1/2} = 2.7 \) wk in river water (Hartley & Kidd 1987; Tomlin 1994).

Ground water:

Sediment:
Soil: duration of activity in soil 1–5 d (Hartley & Kidd 1987; Tomlin 1994);
reported field \( t_{1/2} = 8–144 \) d, recommended field \( t_{1/2} = 5 \) d (Augustijn-Beckers et al. 1994).

Biota:
18.1.1.42 Fensulfothion

Common Name: Fensulfothion
Synonym: Dassnit, Terracur
Chemical Name: O,O-diethyl O-4-methylsulphinylphenyl phosphorothioate
Uses: insecticide/nematicide
CAS Registry No: 115-90-2
Molecular Formula: C₁₁H₁₇O₄PS₂
Molecular Weight: 308.354
Melting Point (°C):
  yellow-brown oil (Spencer 1982; Hartley & Kidd 1987)
  < 25 (Montgomery 1993)
Boiling Point (°C):
  138–141/0.01 mmHg (Hartley & Kidd 1987, Worthing & Walker 1987; Howard 1991)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
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):
  1600 (Spencer 1982)
  2000 (20°C, shake flask, Bowman & Sans 1979, 1983b)
  1540 (Hartley & Kidd 1987; Worthing & Walker 1987)
  1540 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C):
  9.09 × 10⁻³ (Howard 1991)
  6.67 × 10⁻³ (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol):
  1.40 × 10⁻³ (calculated-P/C, Howard 1991)
Octanol/Water Partition Coefficient, log K_{ow}:
  2.23 (shake flask-concn ratio-GC, Bowman & Sans 1983)
  2.23 (Montgomery 1993)
  2.23 (recommended, Sangster 1993)
  2.23 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
  1.46, 0.93 (calculated-K_{ow}, solubility, Howard 1991)
  1.68 (killifish Oryzias latipes, after 48–72 h exposure, Tsuda et al. 1995)
Sorption Partition Coefficient, log $K_{OC}$:

- 1.83, 2.11 (estimated, Howard 1991)
- 1.89 (calculated, Montgomery 1993)
- 2.09–2.57 (Augustijn-Beckers et al. 1994)
- 2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.52 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 3.05, 2.44, 2.15, 2.237, 2.85 (second generation EUROSOILS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 3.053, 2.443, 2.150, 2.237, 2.848 (second generation EUROSOILS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-$k^\prime$ correlation, Gawlik et al. 2000)
- 2.52; 2.94, 2.62 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis: $t_{1/2} = 58–87$ d over pH range of 4.5–8.0 at 25°C in pure water (Howard 1991).
- Biodegradation: field $t_{1/2} = 30$ d (estimated, Augustijn-Becker et al. 1994).
- Biotransformation:
  - Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
    - $k_2 = 0.17$ h$^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

- Air: $t_{1/2} = 7.03$ h for reaction with OH radicals in the atmosphere (Howard 1991).
- Surface water: $t_{1/2} = 58–87$ d in pure water at 25°C over the pH range of 4.5–8.0 (Howard 1991).
- Ground water:
- Sediment:
- Soil: $t_{1/2} < 1$ wk to several weeks in soil (Howard 1991);
  - field $t_{1/2} = 3$ to 182 d and $t_{1/2} = 30$ d (estimated, Augustijn-Becker et al. 1994; Hornsby et al. 1996).
- Biota:
18.1.1.43 Fenthion

Common Name: Fenthion
Synonym: Bay 29493, Baycid, Bayer 9007, Baytex, Baycid, DMTP, Ekalux, ENT 25540, Entex, Lebacid, Lebaycid, Mercaptophos, MPP, NCI-C08651, OMS 2, Queletox, Spotan, Talodox, Tiquvon
Chemical Name: O,O-dimethyl O-(3-methyl-4-(methylthio)phenyl) phosphorothioate; O,O-dimethyl O-4-methylthio-m-tolyl phosphorothioate
Uses: insecticide with contact, stomach and respiratory action and also used as acaricide and cholinesterase inhibitor.
CAS Registry No: 55-38-9
Molecular Formula: C$_{10}$H$_{15}$O$_3$PS$_2$
Molecular Weight: 278.328
Melting Point (°C):
7.0 (Montgomery 1993)
7.5 (Tomlin 1994; Milne 1995)
Boiling Point (°C):
87.0 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm$^3$ at 20°C):
1.246 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.25 (Worthing & Hance 1991; Montgomery 1993)
Molar Volume (cm$^3$/mol):
264.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK$_a$:
89.31 (Rordorf 1989)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
89.31 (Rordorf 1989)
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: 1.0
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
55 (Günther et al. 1968; Martin & Worthing 1977; Budavari 1989)
56 (22°C, Khan 1980)
55 (22°C, Verschueren 1983)
7.51 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
9.3 (20°C, shake flask-GC, Bowman & Sans 1985)
54–56 (20°C, Hartley & Kidd 1987)
2.0 (20°C, Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)
2.0, 4.2, 7.51, 9.3, 50 (20°C, literature data variability, Heller et al. 1989)
4.2 (20°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
$4.0 \times 10^{-3}$ (20°C, Eichler 1965)
$4.0 \times 10^{-3}$ (20°C, Melnikov 1971)
$4.0 \times 10^{-3}$ (20°C, Hartley & Graham-Bryce 1980)
$4.0 \times 10^{-3}$ (20°C, Khan 1980; Budavari 1989; Worthing & Hance 1991; Montgomery 1993)
$8.4 \times 10^{-3}$ (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

- 0.022 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.547 (Montgomery 1993)

Octanol/Water Partition Coefficient, log $K_{OW}$:

- 4.09 (shake flask-GC, Bowman & Sans 1983b)
- 4.167 ± 0.009 (shake flask/slow-stirring method, De Bruijn & Hermens 1991)
- 4.09, 4.84 (RP-HPLC correlation, Saito et al. 1993)
- 4.09 (recommended, Sangster 1993)
- 4.84 (Tomlin 1994)
- 4.09 (selected, Hansch et al. 1995)
- 4.17 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

- 1.81 (calculated-S, Kenaga 1980)
- −4.50 (beef biotransfer factor log $B_p$, correlated-$K_{OW}$, MacDougall 1972)
- −5.60 (milk biotransfer factor log $B_m$, correlated-$K_{OW}$, Johnson & Bowman 1972)
- 4.22 ± 0.08 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
- 4.17 ($Poecilia reticulata$, De Bruijn & Hermens 1991)
- 2.68 (whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
- 1.34, 1.46, 1.43, 1.41 (whole body carp: 24 h, 72 h, 120 h, and 148 h; Tsuda et al. 1993)
- 1.96 (killifish $Oryzias latipes$, after 12–72 h exposure, Tsuda et al. 1995)
- 1.96, 2.02 ($Oryzias latipes$, Tsuda et al. 1995; quoted, Devillers et al. 1996)

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

- 2.68 (calculated-S, Kenaga 1980)
- 3.31 (soil, HPLC-screening test, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995a, b)
- 0.89–1.58 (Montgomery 1993)
- 3.18 (Tomlin 1994; Lohninger 1994)
- 3.31; 3.37 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 3.10 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
- 3.50, 3.00 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis: $t_{1/2} = 223$ d at pH 4, $t_{1/2} = 200$ d at pH 7, and $t_{1/2} = 151$ d at pH 9 at 22°C (Tomlin 1994).
Biodegradation: rate constants $k = -0.00745 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.00199 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.00129 \text{ h}^{-1}$ in nonsterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = (8.81 \pm 0.72) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)
- $k_2 = (0.60 \pm 0.02) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)
- $k_2 = 0.42 \text{ d}^{-1}$ (guppy, calculated-KOW, De Bruijn & Hermens 1991)
- $k_2 = 0.07 \text{ h}^{-1}$ (whole body willow shiner, Tsuda et al. 1992)
- $k_2 = 0.34 \text{ h}^{-1}$ (carp, Tsuda et al. 1992)
- $k_2 = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)
- $k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)
- $k_2 = 0.34 \text{ h}^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:
Air:
Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);
- $t_{1/2} = 189 \text{ d at } 6^\circ \text{C}, 71 \text{ d at } 2.2^\circ \text{C}$ in darkness for Mill-Q water at pH 6.1; $t_{1/2} = 149 \text{ d at } 6^\circ \text{C}$, $t_{1/2} = 42 \text{ d at } 22^\circ \text{C}$ in darkness, $t_{1/2} = 2 \text{ d under sunlight conditions for river water at pH 7.3}$; $t_{1/2} = 104 \text{ d at } 6^\circ \text{C}$, $t_{1/2} = 33 \text{ d at } 22^\circ \text{C}$ in darkness for filtered river water, pH 7.3; $t_{1/2} = 227 \text{ d at } 6^\circ \text{C}$, $t_{1/2} = 26 \text{ d at } 22^\circ \text{C}$ in darkness, $t_{1/2} = 5 \text{ d under sunlight conditions for seawater at pH 8.1}$ (Lartiges & Garrigues 1995).

Ground water:
Soil: selected field $t_{1/2} = 34 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);
- $t_{1/2} \sim 1 \text{ d in soil and water}$ (Tomlin 1994).

Biota: excretion rate constant $k = 0.07 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
- elimination rate constants $k = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH)}$ and $k = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993);
- excretion rate constant $k = 0.34 \text{ h}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ from carp (Tsuda et al. 1993).
18.1.1.44 Fenvalerate

Common Name: Fenvalerate
Synonym: Belmark, Ectrin, Pydrin, Pyrethroid, S 5602, Sanmarton, SD 43775, Sunicide, Sumicidin, Sumifly, Sumipower, WL 43775
Chemical Name: (RS)-α-cyano-3-phenoxybenzyl (RS)-2-(4-chlorophenyl)-3-methylbutyrate; cyano-(3-phenoxyphenyl)methyl 4-chloro-α-(1-methylethyl)benzeneacetate
Uses: non-systemic insecticide to control a wide variety of pests and also used as acaricide
CAS Registry No: 51630-58-1
Molecular Formula: C_{25}H_{22}ClNO_{3}
Molar Formula: C_{25}H_{22}ClNO_{3}
Molar Weight: 419.901
Melting Point (°C): liquid
Boiling Point (°C):
- decomposes on distillation (Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm³ at 20°C):
- 1.26 (22°C, Spencer 1982)
- 1.17 (23°C, Hartley & Kidd 1987; Milne 1995)
Molar Volume (cm³/mol):
- 479.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
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):
- 0.085 (shake flask-GC, Coats & O’Donnell-Jafferey 1979)
- 0.085 (Verschueren 1983; quoted, Pait et al. 1992)
- 0.024 (in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)
- <1.0 (20°C, Worthing 1979, 1987; Spencer 1982)
- <1.0 (20°C, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
- <0.02 (Davies & Lee 1987; quoted, Kawamoto & Urano 1989)
- <1.0 (tech. grade at 20°C, Worthing & Walker 1991)
Vapor Pressure (Pa at 25°C or as indicated):
- 4.90 × 10⁻⁷ (Barlow 1978)
- 3.07 × 10⁻⁵ (Worthing 1979)
- 1.33 × 10⁻⁵ (22°C, Spencer 1982)
- 3.70 × 10⁻⁵ (Hartley & Kidd 1987)
- 1.47 × 10⁻⁶ (Budavari 1989)
- 3.73 × 10⁻⁵ (Kawamoto & Urano 1989)
- 8.10 × 10⁻⁷ (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
- 3.70 × 10⁻⁵ (tech. grade, Worthing & Hance 1991)
- 1.92 × 10⁻⁷ (20°C, Tomlin 1994)
- 1.78 × 10⁻⁶ (solid Pₛ, converted from Pₐ determined by GC-RT correlation, Tsuzuki 2001)
Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
- 0.0152 (20–25°C, calculated-P/C, Montgomery 1993)
- 0.308 (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
- 0.0211 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:
- 4.42 (shake flask-GC, Coats & O’Donnell-Jafferey 1979)
- 6.20 (shake flask-GC, Schimmel et al. 1983)
- 5.2 ± 0.6 (HPLC-RT correlation, Muir et al. 1985)
- 6.65 (shake flask, Log P Database, Hansch & Leo 1987)
- 6.25 (HPLC-RT correlation, Kawamoto & Urano 1989)
- 4.09 (23°C, Worthing & Walker 1991)
- 6.25 (HPLC-RT correlation, Hu& Leng 1992)
- 4.09–6.25 (Montgomery 1993)
- 6.20 (recommended, Sangster 1993)
- 5.01 (23°C, Tomlin 1994)
- 6.20 (recommended, Hansch et al. 1995)
- 4.08 (23°C, Milne 1995)

Bioconcentration Factor, log BCF:
- 3.67 (quoted, Schimmel et al. 1983)
- 1.67–1.84 (sand, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
- 2.01–2.24 (sand, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
- 1.30–1.53 (sand, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
- 1.62–1.87 (silt, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
- 1.36–2.06 (silt, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
- 1.26–1.97 (silt, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
- 1.36–1.51 (clay, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
- 2.09–2.19 (clay, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
- 0.95–1.70 (clay, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
- 4.48, 4.57 (oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
- 4.48, 4.57 (sheephead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
- −3.09 (milk biotransfer factor log B_{m}, correlated-K_{OW}, Wszolek et al. 1980; quoted, Travis & Arms 1988)
- 2.61, 2.96 (Oncorhynchus mykiss, Muir et al. 1994; quoted, Devillers et al. 1996)
- 2.70 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
- 2.58 (silt, reported as K_{p} on 78% DOC, Muir et al. 1985)
- 2.61 (clay, reported as K_{p} on 61% DOC, Muir et al. 1985)
- 1.30 (selected, USDA 1989; quoted, Neary et al. 1993)
- 3.64 (calculated, Montgomery 1993)
- 3.72 (estimated-chemical structure, Lohninger 1994)
- 3.74 (soil, calculated-MCI χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
- Biodegradation: rate constant k(aerobic) = 0.055 d⁻¹ with t_{1/2} = 13 d at 20°C by aerobic activated sludge, and k(anaerobic) = 0.055 d⁻¹ with t_{1/2} = 13 d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

Half-Lives in the Environment:
- Air:
  - Surface water: t_{1/2} = 14 d in 100 mL of a pesticide-seawater solution under outdoor light, t_{1/2} > 14 d under outdoor dark condition and t_{1/2} > 28 d under indoor condition (Schimmel et al. 1983);
\( t_{1/2} = 27-42 \) d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993).

\( t_{1/2} = 13 \) d biodegradation by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990).

Ground water:
Sediment: \( t_{1/2} = 34 \) d in 10 g of sediment/100 mL of a pesticide-seawater solution in untreated condition and
\( t_{1/2} > 28 \) d in sterile condition (Schimmel et al. 1983).
Soil: selected field \( t_{1/2} = 35 \) d (Wauchope et al. 1992; Hornsby et al. 1996).
soil \( t_{1/2} = 50 \) d (Pait et al. 1992).
Biota: average \( t_{1/2} = 35 \) d in the forest (USDA 1989; quoted, Neary et al. 1993).
18.1.1.45 Flucythrinate

Common Name: Flucythrinate
Synonym: AC 222705, Cybolt, Cythrin, Pay-Off
Chemical Name: (RS)-α-cyano-3-phenoxybenzyl(5)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate; cyano(3-phenoxy phenyl)methyl 4-(difluoromethoxy)-α-(1-methylethyl)benzeneacetate
Uses: non-systemic insecticide with contact and stomach action to control a wide range of insect pests in cotton, fruit trees, strawberries, vines, fruits, olives, coffee, cocoa, hops, vegetables, soybeans, cereals, maize, alfalfa, sugar beet, sunflowers and ornamentals
CAS Registry No: 70124-77-5
Molecular Formula: C_{26}H_{23}F_{2}NO_{4}
Molecular Weight: 451.463
Melting Point (°C):
< 25 (dark amber liquid, Montgomery 1993)
Boiling Point (°C):
108.0 (at 0.35 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
1.190 (22°C, Worthing & Hance 1991)
Molar Volume (cm³/mol):
499.9 (calculated-Le Bas method at normal boiling point)
379.4 (22°C, calculated-density)
Dissociation Constant, pKₐ:
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.049 (in seawater, Schimmel et al. 1983)
0.06 (20–25°C, selected, Wauchope 1989; Hornsby et al. 1996)
0.50 (21°C, Montgomery 1993)
Vapor Pressure (Pa at 25°C or as indicated):
1.2 × 10⁻⁶ (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
9.066 (Montgomery 1993)
2.69 × 10⁻⁶, 2.2 × 10⁻⁶ (liquid P_L, GC-RT correlation; Donovan 1996)
1.2 × 10⁻⁶ (20–25°C, selected, Hornsby et al. 1996)
2.82 × 10⁻⁶ (solid P_s, converted from P_L determined by GC-RT correlation method, Tsuzuki 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
8187 (21–25°C, calculated-P/C, 8.08 × 10⁻² atm·m³/mol, Montgomery 1993)
0.0011 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow}:
6.28 (shake flask-GC, Schimmel et al. 1983)
6.20 (Clark et al. 1989)
Bioconcentration Factor, log BCF:
2.96  (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.81  (calculated, Montgomery 1993)
5.00  (20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization:
Photolysis: t_{1/2} ~ 21 d for degradation on soil plates by simulated sunlight and t_{1/2} = 4.0 d in aqueous solutions (Tomlin 1994).
Oxidation:
Hydrolysis: t_{1/2} = 40, 52, and 6.3 d at pH 3, 5, 9 all at 27°C (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).
Biodegradation:
Biotransformation:

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

Half-Lives in the Environment:
Air:
Surface water: t_{1/2} = 34 d in an estuarine environment (Schimmel et al. 1983; quoted, Montgomery 1993).
Ground water:
Sediment:
Soil: t_{1/2} ~ 2 months in soil (Tomlin 1994);
field t_{1/2} = 21 d (20–25°C, selected, Hornsby et al. 1996).
Biota:
18.1.1.46 Fonofos

![Chemical Structure of Fonofos](image)

**Common Name:** Fonofos  
**Synonym:** Difonate, Dyfonate, ENT-25796, Fonophos, N 2788, N-2790, Stauffer NA 2790  
**Chemical Name:** \(O\)-ethyl \(S\)-phenyl \((RS)\)-ethylphosphorodithioate; \((\pm)\)-\(O\)-ethyl \(S\)-phenyl ethylphosphorodithioate

**Uses:** soil insecticide to control rootworms, wireworms, crickets and similar crop pests in vegetables, sorghum, ornamentals, cereals, maize, vines, olives, sugar beet, sugar cane, potatoes, groundnuts, tobacco, turf, and fruit crops  
**CAS Registry No:** 944-22-9 (unstated stereochemistry); 66767-39-3 (racemate); 62705-71-9 \((R)\)-isomer; 62680-03-9 \((S)\)-isomer

**Molecular Formula:** \(C_{10}H_{15}OPS_2\)  
**Molecular Weight:** 246.329

**Melting Point \(^\circ\text{C}\):** liquid  
**Boiling Point \(^\circ\text{C}\):**

- 130 \((\text{at} \ 0.1 \ \text{mmHg}, \ \text{Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995})\)
- 1.160 \((25^\circ\text{C}, \ \text{Hartley & Kidd 1987; Tomlin 1994; Milne 1995})\)
- 1.154 \((\text{Worthing & Hance 1991; Montgomery 1993})\)

**Density \((\text{g/cm}^3\) at \(20^\circ\text{C})\):**

- 1.160 \((25^\circ\text{C}, \ \text{Hartley & Kidd 1987; Tomlin 1994; Milne 1995})\)
- 1.154 \((\text{Worthing & Hance 1991; Montgomery 1993})\)

**Molar Volume \((\text{cm}^3/\text{mol})\):** 213.4 \((\text{calculated-density})\)

**Dissociation Constant, \(pK_a\):**

**Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):**

**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), \(F\): 1.0**

**Water Solubility \((\text{g/m}^3\) or mg/L at 25^\circ\text{C} or as indicated):**

- 13 \((22^\circ\text{C}, \ \text{Spencer 1973})\)
- 13 \((\text{Wauchope 1978})\)
- 15.7 \((20^\circ\text{C}, \ \text{shake flask-GC, Bowman & Sans 1979, 1983b})\)
- 13 \((\text{Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995})\)
- 13 \((20^\circ\text{C}, \ \text{Worthing & Walker})\)
- 16.9 \((20–25^\circ\text{C, selected, Wauchope et al. 1992; Hornsby et al. 1996})\)
- 13 \((\text{rm. temp., Montgomery 1993})\)
- 13 \((22^\circ\text{C}, \ \text{Tomlin 1994})\)

**Vapor Pressure \((\text{Pa} at 25^\circ\text{C} or as indicated):**

- 0.0267 \((\text{Menn 1969; Fuhrmann & Lichtenstein 1980})\)
- 0.028 \((\text{Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994})\)
- 0.028 \((\text{Worthing & Walker 1987; Worthing & Hance 1991})\)
- 0.0453 \((20–25^\circ\text{C, selected, Wauchope et al. 1992; Hornsby et al. 1996})\)

**Henry’s Law Constant \((\text{Pa}\cdot\text{m}^3/\text{mol} at 25^\circ\text{C} or as indicated):**

- 0.5206 \((\text{calculated-P/C as per Worthing & Walker 1987, Schomburg et al. 1991})\)
- 0.5268 \((20–25^\circ\text{C, calculated-P/C, Montgomery 1993})\)
- 0.530 \((\text{calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995})\)

**Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\) at 25^\circ\text{C} or as indicated:**

- 3.892 \((\text{shake flask-GC, Bowman & Sans 1983b})\)
- 3.94 \((\text{shake flsk, Log P Database, Hansch & Leo 1987})\)
- 3.90 \((20^\circ\text{C, Worthing & Hance 1991})\)
3.89, 3.90 (Montgomery 1993)
3.94 (recommended, Sangster 1993)
3.94 (Tomlin 1994)
3.90 (Milne 1995)
3.94 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.89 (mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
2.3–2.7 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
1.83 (screening model calculations, Jury et al. 1987b)
1.18 (loam soil, Worthing & Hance 1991)
2.94 (soil, 20–25°C, selected, Wauchope et al. 1992)
3.03 (calculated, Montgomery 1993)
2.94 (estimated-chemical structure, Lohninger 1994)
2.94 (soil, 20–25°C, selected, Hornsby et al. 1996)
3.44; 3.0, 3.04 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:
Photolysis: t_{1/2} = 12 d in water at pH 5 and 25°C (Worthing & Hance 1991; Tomlin 1994).

Oxidation:
Hydrolysis: alkaline chemical hydrolysis rate constant k = 1 × 10^{-4} M^{-1} s^{-1} with t_{1/2} > 365 d (selected, sediment/water, Schnoor & McAvoy 1981; quoted, Schnoor 1992);
hydrolysis t_{1/2} = 74–127 d in water at 40°C and pH 7, t_{1/2} = 101 d at pH 4 (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994).

Biodegradation:

Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water:
Ground water:

Soil:
Persistence of less than one month in soil (Wauchope 1978);
t_{1/2} > 24 wk in sterile sandy loam and t_{1/2} = 3.0 wk in nonsterile sandy loam;
t_{1/2} > 24 wk in sterile organic soil and t_{1/2} = 4.0 wk in nonsterile organic soil (Miles et al. 1979);
t_{1/2} = 60 d from screening model calculations (Jury 1987b);
t_{1/2} = 16.5–28 d at 24°C (Worthing & Hance 1991);
selected field t_{1/2} = 40 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical t_{1/2} = 60 d from screening model calculations (Jury et al. 1987b).
18.1.147 α-HCH

Common Name: α-HCH
Synonym: α-BHC, α-Hexachlorocyclohexane
Chemical Name: α-1,2,3,4,5,6-hexachlorocyclohexane, (1α, 2α, 3α, 4α, 5β, 6β-1, 2, 3, 4, 5, 6-hexachloro-cyclohexane
CAS Registry No: 319-84-6
Molecular Formula: C₆H₆Cl₆
Molecular Weight: 290.830
Melting Point (°C):
  158  (Lide 2003)
Boiling Point (°C): 288
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  243.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of fusion, ΔHₘₚ (kJ/mol):
  30.96  (Ruelle & Kesselring 1997)
Entropy of fusion, ΔSₘₚ (J/mol K):
  72.0  (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F: 0.0496 (mp at 158°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
  10  (20°C, Slade 1945, Günther et al. 1968; Ulmann 1972; Horvath 1982)
  1.63  (shake flask-GC, Kanazawa et al. 1971)
  2.03, 1.21  (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 µm particle size, Kurihara et al. 1973)
  1.77, 1.48  (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 µm particle size, Kurihara et al. 1973)
  1.21–2.03  (28°C, Kurihara et al. 1973)
  2.0  (generator column-GC/ECD, Weil et al. 1974)
  4.3  (shake flask-GC/ECD, Malayandi et al. 1982)
  1.51  (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
  21.6  (supercooled liquid value, Majewski & Capel 1995)
  0.666, 0.023  (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
log [Sᵢ/(mol/L)] = 2.790 – 1621/(T/K) (supercooled liquid, Passivirta et al. 1999)
  85.22, 96.85  (supercooled liquid values: LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
log Sᵢ/(mol m⁻³) = − 398.5/(T/K) + 0.859 (supercooled liquid, final adjusted eq., Xiao 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):
  2.67*  (20°C, static method, measured range 20–60°C, Slade 1945)
  0.00333*  (20°C, effusion manometer, measured range 15–30°C, Balson 1947)
  0.27  (supercooled liquid value from Balson 1947; quoted, Hinckley et al. 1990)
  0.0073  (20°C, Deutsche Forschungsgemeinschaft 1983; quoted, Ballschmiter & Wittlinger 1991; Fischer et al. 1991; Schreitmüller & Ballschmiter 1995)
  0.0840  (20°C, supercooled liquid value, Bidleman et al. 1986)
  0.313  (GC-RT correlation, Watanabe & Tatsukawa 1989)
  0.227  (supercooled liquid Pᵥ, GC-RT correlation, Hinckley et al. 1990)
log (Pᵥ/Pa) = 10.49 – 3301/(T/K) (supercooled liquid, Hinckley et al. 1990)
log (Pᵥ/Pa) = 11.34 – 3375/(T/K) (supercooled liquid, Hinckley et al. 1990)
  0.003  (selected, Suntio et al. 1988, quoted, Calamari et al. 1991; Schreitmüller & Ballschmiter 1995)
  0.0060  (quoted, Howard 1991)
  0.00647  (quoted, supercooled liquid value, Majewski & Capel 1995)

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log \( P_L / P_a \) = 10.77 – 3335/(T/K) (supercooled liquid, Passivirta et al. 1999)
log \( P_L / P_a \) = –3497/(T/K) + 11.12 (supercooled liquid, final adjusted eq., Xiao et al. 2004)

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

0.47–0.792 (Callahan et al. 1979)
2.16 (gas stripping-GC, Atlas et al. 1982)
0.55 (calculated-P/C, Mabey et al. 1982)
0.87 (calculated-P/C, Suntio et al. 1988)
1.10 (calculated-P/C, Ballcsmiter & Wittlinger 1991; Fischer et al. 1991)
1.07 (calculated-P/C, Howard 1991)
0.43 (calculated-P/C, Calamari et al. 1991)

0.677* (23°C, gas stripping-GC/ECD, distilled water, measured range 0.5–45°C, Kucklick et al. 1991)

log \[ H/(Pa·m³ mol –1) \] = –2969/(T/K) + 9.88, temp range 0.5–45°C (gas stripping-GC measurements, artificial seawater, Kucklick et al. 1991)

0.87 (20°C), 2.40, 1.10, 0.677, 0.710 (23°C) (quoted, Iwata et al. 1993)

0.87 (20°C), 2.40, 1.10, 0.677, 0.710 (23°C) (quoted, Iwata et al. 1993)

0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log \( K_{AW} \) = 5.485 – 2682/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

3.81 (shake flask-GC, Kurihara et al. 1973)
3.81 (HPLC-RT correlation, Sugiura et al. 1979)
3.90 (Veith et al. 1979)
3.776 ± 0.025 (shake flask/slow stirring method; De Bruijn et al. 1989)
3.80 (recommended, Sangster 1993)
3.80 (recommended, Hansch et al. 1995)
3.79* ± 0.001 (shake flask/slow stirring-GC, measured range 5–45°C, Paschke & Schüürmann 1998)
3.81; 4.57 (quoted lit.; calculated, Passivirta et al. 1999)

3.81, 3.94 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)

log \( K_{OW} \) = –374.5/(T/K) + 2.55 (LDV linear regression of literature data, Xiao et al. 2004)
log \( K_{OW} \) = –266.2/(T/K) + 3.04 (LDV linear regression of literature data, Xiao et al. 2004)
Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

6.90 (calculated-\( K_{OW}/K_{AW} \), Wania & Mackay 1996)
7.26 (calculated, Finizio et al. 1997)
log \( K_{OA} = -3.23 + 3231/(T/K) \), temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
7.61, 7.464 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
log \( K_{OA} = 3231/(T/K) – 3.23 \) (LDV linear regression of literature data, Xiao et al. 2004)

Bioconcentration Factor, log BCF:

2.03 (mussels, Ernst 1977; quoted, Renberg & Sundström 1979; Hawker & Connell 1986)
3.08, 2.52, 2.78, 2.77 (golden orfe, carp, brown trout, guppy, Sugiuira et al. 1979)
2.20, 2.82 (mussels, Geyer et al. 1982)
2.97–3.38 mean 3.20; 2.97–3.45 mean 3.38 (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
3.20, 2.85 (rainbow trout: laboratory BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
1.93 (paddy field fish, Soon & Hock 1987)
2.15 (calculated, Isnard & Lambert 1988)
6.01 (azalea leaves, Bacci et al. 1990)
3.04 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991)
2.33 (early juvenile of rainbow trout, Vigano et al. 1992)
5.72 (azalea leaves, calculated, Müller et al. 1994)
2.79; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI \( \chi \), calculated-\( K_{OW} \), Lu et al.1999)
2.33; 2.44 (Onchorhynchus mykiss, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

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

3.81 (calculated-S, Lyman et al. 1982)
4.10, 3.5 (field sediment trap material, calculated-\( K_{OW} \), Oliver & Charlton 1984)
3.25 (av. lit. value, Gerstl 1991)
3.32 (derived from exptl., Meylan et al. 1992)
3.53* (calculated-MCI \( \chi \), Meylan et al. 1992)
3.25 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)
5.50 (soil, calculated-universal solvation model, Winget et al. 2000)

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

Volatilization: volatilization \( t_{\frac{1}{2}} \sim 6 \) d from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Saleh et al. 1982); \( t_{\frac{1}{2}} \sim 500 \) d from a model pond (estimated, Howard 1991).

Photolysis:

Oxidation: photooxidation \( t_{\frac{1}{2}} = 2.3 \) d for reaction with OH radical in the gas phase (Atkinson 1987).

Hydrolysis: hydrolytic \( t_{\frac{1}{2}} = 26 \) yr at pH 8 and 5°C (Ngabe et al. 1993).

Biodegradation: overall degradation rate constant \( k = 0.0648 \) h\(^{-1}\) with \( t_{\frac{1}{2}} = 10.7 \) h for (+)-\( \alpha \)-HCH and rate constant \( k = 0.0298 \) h\(^{-1}\) with \( t_{\frac{1}{2}} = 23.3 \) h for (-)-\( \alpha \)-HCH were calculated from experiments S1–S3 of (35 ± 0.5) h for (+) enantiomer and 99 ± 3.5 h for (-) enantiomer in sewage sludge (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\( k_1 = 3.82 \) h\(^{-1}\); \( k_2 = 0.036 \) h\(^{-1}\) (mussels, Ernst 1977; quoted, Hawker & Connell 1986)
\( k_1 = 0.52 \) d\(^{-1}\), 0.56 d\(^{-1}\), 0.91 d\(^{-1}\), and 0.42 d\(^{-1}\) (golden orfe, carp, brown trout, and guppy at steady state, Sugiuira et al. 1979)
\( k_2 = 0.0009 \) h\(^{-1}\) (azalea leaves, Peterson et al. 1991)
\( k_1 = 27.6 \) h\(^{-1}\); \( k_2 = 0.13 \) h\(^{-1}\) (early juvenile of rainbow trout, Vigano et al. 1992)

Half-Lives in the Environment:

Air: atmospheric \( t_{\frac{1}{2}} \sim 2.3 \) d based on reaction with OH radical at 25°C (Atkinson 1987);
half-lives in the Great Lake’s atmosphere. $t_{1/2} = 4.4 \pm 0.2$ yr at Eagle Harbor, $t_{1/2} = 3.5 \pm 0.2$ yr at Sleeping Bear Dunes and $t_{1/2} = 3.3 \pm 0.2$ yr at Sturgeon Point (Buehler et al. 2004).

Surface water: $t_{1/2} = 1.7$–77 d in various locations in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Ground water:

Sediment:

Soil: $t_{1/2} = 8.2$ and 7.1 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: $t_{1/2} = 19.2$ h (mussels, Ernst 1977).

### TABLE 18.1.1.47.1
Reported vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of $\alpha$-HCH at various temperatures

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Log $K_{OW}$</th>
<th>Log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>static method</td>
<td>eflux-manometer</td>
<td>shake flask/GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>----------------</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>20</td>
<td>2.67</td>
<td>20</td>
</tr>
<tr>
<td>40</td>
<td>8.0</td>
<td>10</td>
</tr>
<tr>
<td>60</td>
<td>44.0</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
</tr>
<tr>
<td></td>
<td></td>
<td>40</td>
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<td>50</td>
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<td>60</td>
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<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\log P = A - B/(T/K)$

$A = 11.950$

$B = 4850$

temp range: 51–71°C

**FIGURE 18.1.1.47.1** Logarithm of vapor pressure versus reciprocal temperature for $\alpha$-HCH.
**FIGURE 18.1.1.47.2** Logarithm of $K_{OW}$ versus reciprocal temperature for $\alpha$-HCH.

**FIGURE 18.1.1.47.3** Logarithm of $K_{OA}$ versus reciprocal temperature for $\alpha$-HCH.
<table>
<thead>
<tr>
<th>T/°C</th>
<th>H/(Pa m^3/mol)</th>
<th>T/°C</th>
<th>H/(Pa m^3/mol)</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>0.5</td>
<td>0.104</td>
<td>8.0</td>
<td>0.215</td>
<td>10</td>
<td>0.17</td>
<td>5</td>
<td>0.094</td>
</tr>
<tr>
<td>10</td>
<td>0.255</td>
<td>18.9</td>
<td>0.491</td>
<td>20</td>
<td>0.43</td>
<td>10</td>
<td>0.15</td>
</tr>
<tr>
<td>23</td>
<td>0.677</td>
<td>18.9</td>
<td>0.491</td>
<td>30</td>
<td>0.92</td>
<td>20</td>
<td>0.38</td>
</tr>
<tr>
<td>35</td>
<td>1.34</td>
<td>18.5</td>
<td>0.373</td>
<td>35</td>
<td>1.52</td>
<td>30</td>
<td>0.79</td>
</tr>
<tr>
<td>45</td>
<td>3.27</td>
<td>18.5</td>
<td>0.373</td>
<td>40</td>
<td>2.21</td>
<td>35</td>
<td>1.32</td>
</tr>
<tr>
<td>eq. 4a</td>
<td>H/(Pa m^3/mol)</td>
<td>eq. 4a</td>
<td>H/(Pa m^3/mol)</td>
<td>eq. 4a</td>
<td>H/(Pa m^3/mol)</td>
<td>eq. 4a</td>
<td>H/(Pa m^3/mol)</td>
</tr>
<tr>
<td>A</td>
<td>9.31</td>
<td>A</td>
<td>10.88 ± 0.50</td>
<td>A</td>
<td>3298 ± 149</td>
<td>A</td>
<td>10.13 ± 0.29</td>
</tr>
<tr>
<td>B</td>
<td>2810</td>
<td>B</td>
<td>3298 ± 149</td>
<td>B</td>
<td>3088 ± 84</td>
<td>B</td>
<td>3088 ± 84</td>
</tr>
</tbody>
</table>

| enthality of transfer air-water ΔH_{AW}(kJ mol⁻¹) = 59.3 |

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FIGURE 18.1.47.4 Logarithm of Henry’s law constant versus reciprocal temperature for α-HCH.

α-HCH: Henry’s law constant vs. 1/T

Kucklick et al. 1991
McConnell et al. 1993
Jantunen et al. 2000
Sahsuvar et al. 2003
Atlas et al. 1982
Abschuh et al. 1999
β-HCH

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Common Name</td>
<td>β-HCH</td>
</tr>
<tr>
<td>Synonym</td>
<td>β-BHC, β-Hexachlorocyclohexane, 1α,2β,3α,4β,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane</td>
</tr>
<tr>
<td>Chemical Name</td>
<td>β-1,2,3,4,5,6-hexachlorocyclohexane</td>
</tr>
<tr>
<td>CAS Registry No</td>
<td>319-85-7</td>
</tr>
<tr>
<td>Molecular Formula</td>
<td>C₆H₆Cl₆</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>290.830</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>309 (Slade 1945; Ballschmiter &amp; Wittlinger 1991)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td></td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td></td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>243.6 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of fusion, ΔHₘ (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of fusion, ΔSₘ (J/mol K)</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ΔSₘ = 56 J/mol K), F:</td>
<td>0.00164 (mp at 309°C)</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):</td>
<td></td>
</tr>
<tr>
<td>5.0</td>
<td>(20°C, Slade 1945; Gunther et al. 1968; Horvath 1982)</td>
</tr>
<tr>
<td>0.70</td>
<td>(20°C, shake flask-GC, Kanazawa et al. 1971)</td>
</tr>
<tr>
<td>0.20, 0.13</td>
<td>(28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 µm particle size, Kurihara et al. 1973)</td>
</tr>
<tr>
<td>0.70</td>
<td>(20°C, Brooks 1974)</td>
</tr>
<tr>
<td>0.24</td>
<td>(generator column-GC/ECD, Weil et al. 1974)</td>
</tr>
<tr>
<td>0.13–0.70</td>
<td>(Callahan et al. 1979)</td>
</tr>
<tr>
<td>2.04</td>
<td>(20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter &amp; Wittlinger 1991; Fischer et al. 1991)</td>
</tr>
<tr>
<td>7.0</td>
<td>(Worthing &amp; Walker 1983)</td>
</tr>
<tr>
<td>69.5</td>
<td>(supercooled liquid value, Majewski &amp; Capel 1995)</td>
</tr>
<tr>
<td>344, 418.8</td>
<td>(supercooled liquid: derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)</td>
</tr>
<tr>
<td>log [S_L/(mol m⁻³)] = –110.1/(T/K) – 0.211 (supercooled liquid, final adjusted eq., Xiao et al. 2004)</td>
<td></td>
</tr>
<tr>
<td>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):</td>
<td></td>
</tr>
<tr>
<td>0.67*</td>
<td>(20°C, static method, measured range 20–60°C, Slade 1945)</td>
</tr>
<tr>
<td>3.73 × 10⁻⁵*</td>
<td>(20°C, effusion-manometer, measured range 0–110°C, Balson 1947)</td>
</tr>
<tr>
<td>4.90 × 10⁻⁵</td>
<td>(20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter &amp; Wittlinger 1991; Fischer et al. 1991)</td>
</tr>
<tr>
<td>0.266</td>
<td>(GC-RT correlation, Watanabe &amp; Tatsukawa 1989)</td>
</tr>
<tr>
<td>0.0272</td>
<td>(supercooled liquid value, Majewski &amp; Capel 1995)</td>
</tr>
<tr>
<td>0.062, 0.0525</td>
<td>(supercooled liquid P_L LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)</td>
</tr>
<tr>
<td>log (P_L/Pa) = –3563/(T/K) + 10.74 (supercooled liquid, linear regression of literature data, Xiao et al. 2004)</td>
<td></td>
</tr>
<tr>
<td>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):</td>
<td></td>
</tr>
<tr>
<td>0.055</td>
<td>(20–25°C, Mabey et al. 1982)</td>
</tr>
<tr>
<td>0.120</td>
<td>(calculated-P/C, Suntio et al. 1988)</td>
</tr>
<tr>
<td>0.070</td>
<td>(calculated-P/C, Ballschmiter &amp; Wittlinger 1991; Fischer et al. 1991)</td>
</tr>
<tr>
<td>0.0446</td>
<td>(wetted-wall column-GC, Altschuh et al. 1999)</td>
</tr>
</tbody>
</table>

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0.022* (dynamic headspace-GC, measured range 5–35°C, Sahsuvar et al. 2003)

\[
\log \left[ \frac{H}{(Pa \cdot m^3/mol)} \right] = 9.96 - 3400/(T/K), \text{ temp range 5–35°C (dynamic headspace-GC, Sahsuvar et al. 2003)}
\]

0.037, 0.037 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

\[
\log \left[ \frac{H}{(Pa \cdot m^3/mol)} \right] = -3454/(T/K) + 10.16 \quad (LDV \text{ linear regression of literature data, Xiao et al. 2004})
\]

0.042, 0.043 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

\[
\log \left[ \frac{H}{(Pa \cdot m^3/mol)} \right] = -3673/(T/K) + 10.89 \quad (FAV \text{ final adjusted eq., Xiao et al. 2004})
\]

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:

- 3.80 (shake flask-GC, Kurihara et al. 1973)
- 4.15 (HPLC-RT correlation, Sugiura et al. 1979)
- 3.842 ± 0.036; 3.78 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
- 3.81 (recommended, Sangster 1993)
- 3.78 (recommended, Hansch et al. 1995)
- 3.88* ± 0.01 (shake flask/slow stirring-GC, measured range 5–25°C, Paschke & Schüürmann 1998)
- 3.84, 3.92 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

\[
\log K_{OW} = 847.5/(T/K) + 1.07 \quad (LDV \text{ linear regression of literature data, Xiao et al. 2004})
\]

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:


\[
\log K_{OA} = -7.69 + 4937/(T/K), \text{ temp range 5–35°C, (gas saturation-GC, Shoeib & Harner 2002)}
\]

- 8.87, 8.74 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

\[
\log K_{OA} = 4937/(T/K) - 7.69 \quad (LDV \text{ linear regression of literature data, Xiao et al. 2004})
\]

\[
\log K_{OA} = 4391/(T/K) - 5.98 \quad (FAV \text{ final adjusted eq., Xiao et al. 2004})
\]

Bioconcentration Factor, log $BCF$:

- 2.99, 2.44, 2.82, 3.17 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
- 3.08, 2.26, 2.62 (activated sludge, algae, golden ide, reported as log BF, Freitag et al. 1985)
- 2.66 (calculated, Isnard & Lambert 1988)
- 3.16, 3.18 (Brachydanio rerio, flow-through conditions, Butte et al. 1991; quoted, Devillers et al. 1996)
- 2.86; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI $\chi$, calculated-$K_{OW}$, Lu et al.1999)
- 2.50; 2.44 (Oncorhynchus mykiss, wet wt. basis: quoted exp.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

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

- 3.36 (av. lit. value, Gerstl 1991)
- 3.98 (soil, calculated-S as per Kenaga 1980, this work)
- 3.50 (derived from exp., Meylan et al. 1992)
- 3.53 (calculated-MCI $\chi$, Meylan et al. 1992)
- 3.36 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 5.50; 3.50 (soil, calculated-universal solvation model; quoted exp., Winget et al. 2000)

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

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
- Biodegradation: calculated $t_{\frac{1}{2}} = 178$ h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
  - $k_1 = 0.46$ d$^{-1}$, 0.33 d$^{-1}$, 0.53 d$^{-1}$, and 0.18 d$^{-1}$ (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)

Half-Lives in the Environment:
**TABLE 18.1.1.48.1**
Reported vapor pressures and Henry’s law constants of β-HCH at various temperatures

<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>Slade 1945 static method</td>
<td>Balson 1947 effusion manometer</td>
</tr>
<tr>
<td>20</td>
<td>0.667</td>
<td>1.733 × 10⁻⁶</td>
</tr>
<tr>
<td>40</td>
<td>22.7</td>
<td>8.399 × 10⁻⁶</td>
</tr>
<tr>
<td>60</td>
<td>77.3</td>
<td>3.733 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.533 × 10⁻⁴</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.60 × 10⁻⁴</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.907 × 10⁻³</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.00 × 10⁻³</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ln H = A – B/(t/K)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A 11.790</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B 5375</td>
</tr>
<tr>
<td></td>
<td></td>
<td>temp range: 95–117°C</td>
</tr>
</tbody>
</table>

**FIGURE 18.1.1.48.1** Logarithm of vapor pressure versus reciprocal temperature for β-HCH.
FIGURE 18.1.1.48.2 Logarithm of Henry’s law constant versus reciprocal temperature for β-HCH.

TABLE 18.1.1.48.2
Reported octanol-water and octanol-air partition coefficients of β-HCH at various temperatures

<table>
<thead>
<tr>
<th>log K_{OW}</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paschke &amp; Schüürmann 1998</td>
<td>Shoib &amp; Harner 2002</td>
</tr>
<tr>
<td>shake flask-GC</td>
<td>generator column-GC/MS</td>
</tr>
</tbody>
</table>

<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>3.99</td>
<td>5</td>
<td>10.0686</td>
</tr>
<tr>
<td>25</td>
<td>3.88</td>
<td>15</td>
<td>9.4375</td>
</tr>
<tr>
<td>45</td>
<td>3.87</td>
<td>20</td>
<td>8.9875</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25</td>
<td>8.9651</td>
</tr>
</tbody>
</table>

enthalpy of phase transfer:

\[ \Delta H_{OW} / (kJ \text{ mol}^{-1}) = \text{--}8.20 \]

entropy of phase transfer:

\[ \Delta S_{OW} / (J \text{ K}^{-1} \text{ mol}^{-1}) = 62.7 \]

\[ \log K_{OA} = A + B/(T/K) \]

A = 7.692

B = 4937

enthalpy of phase change

\[ \Delta H_{OA} / (kJ \text{ mol}^{-1}) = 94.5 \]
FIGURE 18.1.1.48.3 Logarithm of $K_{OW}$ versus reciprocal temperature for $\beta$-HCH.

FIGURE 18.1.1.48.4 Logarithm of $K_{OA}$ versus reciprocal temperature for $\beta$-HCH.
18.1.1.49  δ-HCH

Common Name: δ-HCH
Synonym: δ-BHC, δ-Hexachlorocyclohexane, 1α,2α,3α,4β,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane
Chemical Name: δ-1,2,3,4,5,6-hexachlorocyclohexane
CAS Registry No: 319-86-8
Molecular Formula: C₆H₆Cl₆
Molecular Weight: 290.830
Melting Point (°C):
141.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
243.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₕₚ (kJ/mol):
21.34 (DSC method, Plato 1972)
21.50 (Ruelle & Kesselring 1997)
Entropy of fusion, ΔSₕₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕₚ = 56 J/mol K), F: 0.0719 (mp at 141.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
10 (20°C, Slade 1945)
15.7, 10.7 (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μm particle size, Kurihara et al. 1973)
11.6, 8.64 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 μm particle size, Kurihara et al. 1973)
8.64–31.4 (shake flask-GC, Kurihara et al. 1973)
10 (20°C, quoted, Günther et al. 1968)
21.3 (20°C, shake flask-GC, Kanazawa et al. 1971)
31.4 (generator column-GC/ECD, Weil et al. 1974)
9.01 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2.67* (20°C, static method, measured range 20–60°C, Slade 1945)
2.27 × 10⁻³* (20°C, effusion manometer, Balson 1947)
0.150 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0309 (supercooled liquid value, Majewski & Capel 1995)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.018 (20–25°C, Mabey et al. 1982)
0.073 (calculated-P/C, Suntio et al. 1988)
0.0825 (calculated-P/C₁, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log Kₐw at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
4.14 (shake flask-GC, Kurihara et al. 1973)
4.14 (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:


log $K_{OA} = -7.45 + 4856/(T/K)$, temp range 5–35°C (gas saturation-GC, Shoeib & Harner 2002)

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

2.82 (soil, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$;

Biodegradation: calculated $t_{1/2} = 126$ h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).

Half-Lives in the Environment:

### TABLE 18.1.1.49.1

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>static method</td>
<td>effusion manometer</td>
<td>shake flask-GC</td>
<td>generator column-GC/MS</td>
</tr>
<tr>
<td>20</td>
<td>2.67</td>
<td>0.02946</td>
<td>0.09466</td>
<td>0.7866</td>
</tr>
<tr>
<td>40</td>
<td>12.0</td>
<td>5.466 × 10⁻⁴</td>
<td>2.266 × 10⁻³</td>
<td>8.533 × 10⁻³</td>
</tr>
<tr>
<td>60</td>
<td>45.33</td>
<td>2.13 × 10⁻¹</td>
<td>5.466 × 10⁻³</td>
<td>2.266 × 10⁻³</td>
</tr>
</tbody>
</table>

log $P = A - B/(T/K)$

$T$ in °C, $P$ in mmHg

A: 12635

B: 5100

temp range: 55–75°C

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FIGURE 18.1.1.49.1 Logarithm of vapor pressure versus reciprocal temperature for δ-HCH.

FIGURE 18.1.1.49.2 Logarithm of $K_{OW}$ versus reciprocal temperature for δ-HCH.
FIGURE 18.1.1.49.3 Logarithm of $K_{OA}$ versus reciprocal temperature for δ-HCH.
Common Name: Heptachlor
Chemical Name: 1, 4, 5, 6, 7, 8, 8-heptachloro-3a, 4, 7, 7a-tetrahydro-4, 7-methanoindene; 3–4, 5, 6, 7, 8, 8a-heptachlorodicyclopentadiene
Uses: non-systemic insecticide with contact, stomach, and some respiratory action to control termites, ants, and soil insects in cultivated and uncultivated soils; also used to control household insects
CAS Registry No: 76-44-8
Molecular Formula: C_{10}H_5Cl_7
Molecular Weight: 373.318
Melting Point (°C): 95.5 (Lide 2003)
Boiling Point (°C): 135–145 (at 1–1.5 mmHg, Montgomery 1993; Tomlin 1994)
Density (g/cm³ at 20°C): 1.65–1.67 (25°C, Hartley & Kidd 1987; Tomlin 1994)
1.66 (Montgomery 1993)
Molar Volume (cm³/mol): 308.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKᵢₐ:
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
73.06 (Rordorf 1989)
Enthalpy of Fusion, ΔHₓₜₕ (kJ/mol):
22 (Rordorf 1989)
22.97 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔSₓₜₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₓₜₕ = 56 J/mol K), F: 0.203 (mp at 95.5°C)
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):
0.056 (25–29°C, shake flask-GC, Park & Bruce 1968)
0.03, 0.125, 0.180* (particle size: 0.01, 0.05 & 5.0µ, shake flask-GC, measured range 15–45°C, Biggar & Riggs 1974)
0.03 (Martin & Worthing 1977; Kenaga 1980a, b; Kenaga & Goring 1980)
<1.0 (Wauchope 1978)
0.056 (Hartley & Graham-Bryce 1980; Worthing & Walker 1987; Hartley & Kidd 1987)
0.05 (Khan 1980)
0.30 (Herbicide Handbook 1983)
0.18 (Montgomery 1993)
0.056 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.307, 1.307 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
log [Cᵢ/(mol m⁻³)] = –770/(T/K) + 0.13 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)
Vapor Pressure (Pa at 25°C or as indicated or reported temperature dependence equations):

- 0.025 (Bowery 1964)
- 0.040 (Eichler 1965; Martin 1972; Quellette & King 1977)
- 0.021 (20°C, Hartley & Graham-Bryce 1980)
- 0.053 (Spencer 1982; Worthing 1983, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 0.0213 (20°C, selected exptl. value, Kim 1985)
- 0.021, 0.410, 5.10, 46, 320 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- log (P_v/P_a) = 14.977 – 4966.6/(T/K); measured range 36.4–95.6°C (solid, gas saturation-GC, Rordorf 1989)
- log (P_v/P_a) = 11.811 – 3816.5/(T/K); measured range 96.6–151°C (liquid, gas saturation-GC, Rordorf 1989)
- 0.031 (supercooled liquid P_v value, GC-RT correlation, Hinckley et al. 1990)
- log (P_v/P_a) = 11.88 – 3995/(T/K) (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
- 0.022 (20°C, selected, Taylor & Spencer 1990)
- 0.040 (20°C, Montgomery 1993)
- 0.0533 (20–25°C, selected, Taylor & Spencer 1990)
- log (P_v/P_a) = –3870/(T/K) + 12.11 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

- 150 (gas stripping-GC, Warner et al. 1987)
- 154 (WERL Treatability Database, Ryan et al. 1988)
- 112 (20°C, calculated-P/C, Suntio et al. 1988)
- 845.4 (calculated-P/C, Jury et al. 1990)
- 17.8 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
- 233 (Montgomery 1993)
- 29.75 (wetted wall column-GC, Altschuh et al. 1999)
- 30, 38 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

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

- 5.44 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1983)
- 3.87 (quoted, Rao & Davidson 1980)
- 5.27 (HPLC-RT correlation, McDuffie 1981)
- 4.40–5.50 (Montgomery 1993)
- 5.27, 5.58 (quoted, Hansch et al. 1995)
- 6.02 (shake flask/slow stirring-GC, Simpson et al. 1995)
- 5.24 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 6.10, 5.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{oa} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- log K_{oa} = –3.95 + 3455/(T/K), temp range 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
- 7.64, 7.76 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

- –1.81 (beef biotransfer factor log B_b, correlated-K_{ow}, Kenaga 1980)
- –1.48 (vegetation, correlated-K_{ow}, Lichtenstein 1960; Nash 1974)
- –2.49 (milk biotransfer factor log B_m, correlated-K_{ow}, Saha 1969)
- 4.26 (oysters, wet wt. basis, Wilson 1963)
- 3.26 (bluegill, field tests, Andrews et al. 1966)
- 3.41 (soft clam, Butler 1971)
- 3.45–4.33 (estuarine fish for 96-h exposure, Schimmel et al. 1976)
- 3.76–3.92 (spot fish, whole body 24-d exposure, Schimmel et al. 1976)
- 3.67 (spot fish, edible tissue 24-d exposure, Schimmel et al. 1976)
- 3.58 (mosquito fish, Callahan et al. 1979)
- 3.56, 3.87 (spot fish for 72-h test, 96-h test. Callahan et al. 1979)
4.57, 4.32 (snails, algae, Callahan et al. 1979)
3.98, 4.30 (fathead minnow, 32-d exposure, 276-d exposure, Veith et al. 1979, 1980)
4.30 (sheepshead minnow, Veith et al. 1979)
4.24, 3.33 (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
3.65, 3.90 (estimated-S, K_{OW}, Bysshe 1982)
3.11–3.56 (earthworm, Gish & Hughes 1982)
3.98, 4.30 (fathead minnow, Veith & Kosian 1983)
4.03 (clam fat, 60-d expt., Hartley & Johnson 1983)
4.26 (oysters, Biddinger & Gloss 1984)
3.90, 3.90, 3.90 (oyster, pinfish, sheepshead minnow, Zaroogian et al. 1985)
4.30, 4.33 (measured for fathead minnow, sheepshead minnow, Zaroogian et al. 1985)
3.93 (oyster, Zaroogian et al. 1985)
3.98 (calculated, Isnard & Lambert 1988)
4.11 (selected, Chessells et al. 1992)
4.48 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
4.38 (screening model calculations, Jury et al. 1987b)
4.34 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
3.81 (Jury et al. 1990)
5.21 (estimated-QSAR and SPARC, Kollig 1993)
4.38 (Montgomery 1993)
4.76 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_\text{1/2}:
Volatileization: measured rate constant k = 3.0 d^{-1} (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989); calculated rate constant k = 5.0 d^{-1} (Glotfelty et al. 1989).

Oxidation: t_\text{1/2} = 5.2–51.7 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order t_\text{1/2} = 23.1 h, based on rate constant k = 2.97 \times 10^{-2} h^{-1} at pH 7.0 and 25°C (Demayo 1972; quoted, Callahan et al. 1979; Kollig et al. 1987; Howard et al. 1991); rate constant k = 61 yr^{-1} at pH 7.0 and 25°C (Kollig 1993)

Biodegradation: aqueous aerobic t_\text{1/2} = 360–1567 h, based on unacclimated aerobic soil grab sample test data (Castro & Yoshida 1971; quoted, Howard et al. 1991); rate constant k = 0.011 d^{-1} by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982; estimated t_\text{1/2} = 220 d in soil (Jury et al. 1990); aqueous anaerobic t_\text{1/2} = 1440–6268 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991)

Half-Lives in the Environment:
Air: t_\text{1/2} = 9.8–59.0 h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).
Surface water: persistence up to 2 wk in river water (Eichelberger & Lichtenberg 1971);
\( t_{1/2} = 38 \text{ d} \) in surface waters in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)
\( t_{1/2} = 23.1–129.4 \text{ h} \), based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991)
Biodegradation \( t_{1/2}(\text{aerobic}) = 15 \text{ d} \), \( t_{1/2}(\text{anaerobic}) = 60 \text{ d} \), hydrolysis \( t_{1/2} = 5.4 \text{ d} \) at pH 2, \( t_{1/2} = 0.96 \text{ d} \) at pH 7 in natural waters (Capel & Larson 1995).
Ground water: \( t_{1/2} = 23.1–129.4 \text{ h} \), based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment:
Soil: \( t_{1/2} \approx 2–5 \text{ yr} \) persistence in soil (Nash & Woolson 1967);
estimated persistence of 2 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
Best estimated \( t_{1/2} = 0.91 \text{ yr} \), true value is between 0.86–0.97 yr when heptachlor was incorporated to 7.5 cm depth in an experimental field (Freeman et al. 1975)
persistence of >24 months (Wauchope 1978);
\( t_{1/2} < 10 \text{ d} \) and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
first-order \( t_{1/2} = 63 \text{ d} \) from biodegradation rate constant \( k = 0.011 \text{ d}^{-1} \) by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);
field \( t_{1/2} = 0.3 \text{ d} \) in moist fallow soil (Glotfelty 1981; quoted, Nash 1983);
microagroecosystem \( t_{1/2} = 3 \text{ d} \) in moist fallow soil (Nash 1983);
measured dissipation rate \( k = 0.28 \text{ d}^{-1} \) (Nash 1983; quoted, Nash 1988);
estimated dissipation rate \( k = 1.0 \) and 0.20 d\(^{-1}\) (Nash 1988);
reported \( t_{1/2} = 9–10 \text{ months} \) in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);
\( t_{1/2} = 23.1–129.4 \text{ h} \), based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991);
estimated biodegradation \( t_{1/2} = 220 \text{ d} \) in soil (Jury et al. 1990);
selected field \( t_{1/2} = 250 \text{ d} \) (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
\( t_{1/2} = 9–10 \text{ months} \) when used at agricultural rates (Tomlin 1994)
\( t_{1/2} = 7–14 \text{ yr} \) in soil (Geyer et al. 2000)

Biota: biochemical \( t_{1/2} = 2000 \text{ d} \) from screening model calculations (Jury et al. 1987b).

### TABLE 18.1.1.50.1
Reported aqueous solubilities and octanol-air partition coefficients of heptachlor at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility</th>
<th>Octanol-air partition coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Biggar &amp; Riggs 1974</td>
<td>Shoeib &amp; Harner 2002</td>
</tr>
<tr>
<td></td>
<td>shake-flask-GC</td>
<td>generator column-GC/MS</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility</th>
<th>Octanol-air partition coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>S/g·m(^{-3})</td>
<td>log K(_{OA})</td>
</tr>
<tr>
<td>15</td>
<td>0.01μ</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.030</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>0.490</td>
<td></td>
</tr>
</tbody>
</table>

\[
\log K_{OA} = A + B/(T/K)
\]

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility</th>
<th>Octanol-air partition coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>8.5093</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>8.2625</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>7.9873</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>7.7934</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>7.7046</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>7.7046</td>
<td></td>
</tr>
</tbody>
</table>

Enthalpy of phase change:

\[
\Delta H_{OA} (kJ mol\(^{-1}\)) = 66.2
\]
FIGURE 18.1.150.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for heptachlor.

FIGURE 18.1.150.2 Logarithm of $K_{OA}$ versus reciprocal temperature for heptachlor.
18.1.1.51 Heptachlor epoxide

Common Name: Heptachlor epoxide
Synonym: β-Heptachlorepoxide, Epoxyheptachlor, HCE, Velsicol 53-CS-17
Chemical Name: 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methanoindan; 2,3,4,5,7,8-hexa-hydro-2,5-methano-2H-indeno(1,2b)oxirene
Uses: a degradation product of heptachlor
CAS Registry No: 1024-57-3
Molecular Formula: C_{10}H_{5}Cl_{7}O
Molecular Weight: 389.317
Melting Point (°C):
160 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
317.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.506 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
61.56 (Plato 1972)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0474 (mp at 160°C)

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):
0.035 (25–29°C, shake flask-GC, Park & Bruce 1968)
0.025, 0.120, 0.20* (shake flask-GC, particle size: 0.01, 0.05 and 5.0µ, measured range 15–45°C, Biggar & Riggs 1974)
0.35 (generator column-GC/ECD, Weil et al. 1974)
0.20–0.35 (Mills et al. 1982; Mabey et al. 1982)
0.90 (Zaroogian et al. 1985)
0.275 (Montgomery 1993)
5.91 (supercooled liquid value, 20–25°C, Majewski & Capel 1995)
0.60, 0.0004 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
7.0, 5.06 (supercooled liquid: LDV derivation of literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):
0.045 (estimated, Mabey et al. 1982)
0.00256 (estimated, Howard 1991)
3.47 × 10⁻⁴ (20°C, Montgomery 1993)
0.0997 (supercooled liquid value, 20–25°C, Majewski & Capel 1995)
0.013, 0.022 (supercooled liquid P_i; LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
395 (calculated-P/C, Mabey et al. 1982)
3.42 (gas-stripping, Warner et al. 1987)
3.25 (Montgomery 1993)
Insecticides

2.13  (wetted-wall column-GC, Altschuh et al. 1999)
2.1, 1.7  (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.43</td>
<td>Briggs 1981</td>
</tr>
<tr>
<td>5.40</td>
<td>(HPLC-RT correlation, Veith et al. 1979)</td>
</tr>
<tr>
<td>4.56 ± 0.05</td>
<td>(shake flask, Noegrohati &amp; Hammers 1992)</td>
</tr>
<tr>
<td>3.65</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>5.40, 5.42</td>
<td>(LDV literature-derived value, FAV final-adjusted value, Shen &amp; Wania 2005)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{oa}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.62, 8.59</td>
<td>(LDV literature-derived value, FAV final-adjusted value, Shen &amp; Wania 2005)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.30, 4.90, 3.78</td>
<td>(algae, snail, mosquito-microcosm expt., Lu &amp; Metcalf 1975)</td>
</tr>
<tr>
<td>3.23</td>
<td>(mussel, Ernst 1977)</td>
</tr>
<tr>
<td>4.16</td>
<td>(fathead minnows, 32-d flow-through aquarium, Veith et al. 1979)</td>
</tr>
<tr>
<td>2.03</td>
<td>(microorganism, calculated-$K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>3.37</td>
<td>(clam fat, 60-d expt., Hartley &amp; Johnson 1983)</td>
</tr>
<tr>
<td>2.93</td>
<td>(oyster, Zaroogian et al. 1985)</td>
</tr>
<tr>
<td>3.87, 3.89</td>
<td>(sheepshead minnow, pinfish, mussel and oyster, Zaroogian et al. 1985)</td>
</tr>
<tr>
<td>−1.45</td>
<td>(beef biotransfer factor log $B_{b}$, correlated-$K_{ow}$, Travis &amp; Arms 1988)</td>
</tr>
<tr>
<td>3.88</td>
<td>(calculated-$K_{ow}$, Howard 1991)</td>
</tr>
<tr>
<td>&gt;4.16, &gt;5.14</td>
<td>(fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)</td>
</tr>
<tr>
<td>4.16; 4.10</td>
<td>(<em>Oncorhynchus mykiss</em>, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.34</td>
<td>(sediment, calculated-$K_{ow}$, Mabey et al. 1982)</td>
</tr>
<tr>
<td>2.00</td>
<td>(bentonite clay, Hill &amp; McCarty 1967)</td>
</tr>
<tr>
<td>4.0–4.3</td>
<td>(suspended solids in river, Frank 1981)</td>
</tr>
<tr>
<td>3.89</td>
<td>(calculated-S, Howard 1991)</td>
</tr>
<tr>
<td>4.32</td>
<td>(calculated, Montgomery 1993)</td>
</tr>
<tr>
<td>3.98</td>
<td>(activated carbon-water, Blum et al. 1994)</td>
</tr>
</tbody>
</table>

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

Volatilization: $t_{1/2} = 60$ h from a model river (Howard 1991).

Photolysis: Oxidation: oxidation rate Constants, $k < 3600$ M$^{-1}$ h$^{-1}$ for reaction with singlet oxygen, and $k = 20$ M$^{-1}$ h$^{-1}$ for reaction with peroxy radical (Mabey et al. 1982) $t_{1/2} = 6–60$ h, based on estimated photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: not expected to be important (Howard et al. 1991)

Biodegradation: $t_{1/2} \sim 25$ d under anaerobic conditions when incubated with thick digester sludge at 35°C (Howard 1991) $t_{1/2}$ (aerobic) = 792–13248 h, based on aerobic soil grab sample data; $t_{1/2}$ (anaerobic) = 24–168 h, based on soil and freshwater mud grab sample data (Howard et al. 1991) $t_{1/2}$ (aerobic) = 33 d, $t_{1/2}$ (anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Biotransformation: rate constant for bacterial transformation in water $k = 3 \times 10^{-12}$ mL cell$^{-1}$ h$^{-1}$ (Mabey et al. 1982). Bioconcentration, Uptake ($k_{u}$) and Elimination ($k_{e}$) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 1.5$ d for vapor-phase reaction with photochemically produced hydroxyl radical (Howard 1991) $t_{1/2} = 6–60$ h, based on estimated photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2} = 35$ d in lower Rhine River in case a first order reduction process may be assumed (Zoeteman 1980)
\( t_{1/2} = 792-13248 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation \( t_{1/2,\text{aerobic}} = 33 \) d, \( t_{1/2,\text{anaerobic}} = 1 \) d in natural waters (Capel & Larson 1995)

Ground water: \( t_{1/2} = 24-26496 \) h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

Sediment:

Soil: \( t_{1/2} = 792-13248 \) h, based on aerobic soil grab sample data (Howard et al. 1991)

\( t_{1/2} \sim 3 \) yr in soil (Geyer et al. 2000)

Biota:

**TABLE 18.1.51.1**

Reported aqueous solubilities of heptachlor epoxide at various temperatures

<table>
<thead>
<tr>
<th>Biggar &amp; Riggs 1974</th>
<th>shake flask-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>( S/g·m^{-3} )</td>
</tr>
<tr>
<td>particle size 0.01µ</td>
<td>0.01</td>
</tr>
<tr>
<td>15</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.025</td>
</tr>
<tr>
<td>35</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 18.1.51.1** Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for heptachlor epoxide.
18.1.1.52 Kepone

Common Name: Kepone
Synonym: Chlordecone, CIBA 8514
Chemical Name: 1,2,3,4,5,6,7,9,10,10-dodecachlorooctahydro-1,3,4-metheno-2-cyclobuta-[c,d]-pentalone
CAS Registry No: 143-50-0
Uses: Insecticide/Fungicide
Molecular Formula: C\textsubscript{10}Cl\textsubscript{10}O
Molecular Weight: 490.636
Melting Point (°C):
\[ 350 \text{ (dec. Howard 1991; Montgomery 1993; Lide 2003)} \]
Boiling Point (°C):
Density (g/cm\textsuperscript{3} at 20°C):
Molar Volume (cm\textsuperscript{3}/mol):
\[ 369.9 \text{ (calculated-Le Bas method at normal boiling point)} \]
Dissociation Constant, pK\textsubscript{a}:
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: \( 6.5 \times 10^{-4} \) (mp at 350°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
\[ 4.0 \text{ (100°C, Günther et al. 1968)} \]
\[ 2.7 \text{ (quoted Weil 1978 unpublished result, Kilzer et al. 1979)} \]
\[ 3.0 \text{ (20°C, Kenaga & Goring 1978, Kenaga 1980)} \]
\[ 7.6 \text{ (24°C, shake flask-nephelometry/fluo., Hollifield 1979; quoted, Howard 1991; Montgomery 1993)} \]
Vapor Pressure (Pa at 25°C):
\[ 3.0 \times 10^{-5} \text{ (Kilzer et al. 1979; quoted, Howard 1991; Montgomery 1993)} \]
Henry’s Law Constant (Pa-m\textsuperscript{3}/mol):
\[ 0.00153 \text{ (calculated-P/C, Howard 1991)} \]
\[ 0.00311 \text{ (calculated-P/C, Montgomery 1993)} \]
\[ 0.00140 \text{ (calculated-P/C, this work)} \]
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
\[ 5.50 \text{ (Di Toro 1985)} \]
\[ 5.41 \text{ (shake flask, log P database, Hansch & Leo 1987)} \]
\[ 4.07 \text{ (calculated, Montgomery 1993)} \]
\[ 5.41 \text{ (recommended, Sangster 1993)} \]
\[ 5.44 \text{ (selected, Hansch et al. 1995)} \]
Bioconcentration Factor, log \( BCF \):
\[ 4.04 \text{ (shrimp, 10–20 d exposure, Bahner et al. 1979)} \]
\[ 3.92 \text{ (Kenaga & Goring 1980)} \]
\[ 4.0, 2.65, 2.76 \text{ (sludge, algae, golden ide, Freitag et al. 1985)} \]
\[ 3.84 \text{ (oyster, Zaroogian et al. 1985)} \]
\[ 4.39, 4.46 \text{ (oyster, calculated-\( K_{\text{OW}} \) & models, Zaroogian et al. 1985)} \]
4.39, 4.47  (sheephead minnow, calculated-$K_{OW}$ & models, Zaroogian et al. 1985)

3.85  (Spot Leiostomus xanthurus, 19-d uptake and 28-d clearance studies, Fisher et al. 1986)

4.11  (grass shrimp Palaemonetes pugio, 16-d uptake and 21-d clearance studies, Fisher & Clark 1990)

3.04–3.34  (fathead minnow, quoted, Howard 1991)

3.19, 3.09, 2.84, 0.91  (Cyprinodon variegatus, Leiostomus xanthurus, Palaemonetes pugio, Callinete sapidus, quoted, Howard 1991)


4.34–4.78  (Atlantic silversides, Howard 1991)

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

3.38–3.41  (calculated, Howard 1991)

4.74  (calculated, Montgomery 1993)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:

Volatilization: $t_\text{½} = 3.8–46$ yr predicted for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1991).

Photolysis: indefinite in air (Howard et al. 1991).

Oxidation:

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aerobic aqueous $t_\text{½} = 7488$ to 17,280 h (312 d to 2 yr), based on aerobic aquatic microcosm study, anaerobic $t_\text{½} = 29,952–69,120$ h (1248 d to 8 yr) based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Kinetic data of spot Leiostomus xanthurus in 19-d uptake and 28-d clearance studies (Fisher et al. 1986)

$k_1 = 0.273$ d$^{-1}$; $k_2 = 0.037$ d$^{-1}$ with $t_\text{½} = 18.7$ d, uncontaminated water + 4% ration contaminated food,

$k_1 = 217.3$ d$^{-1}$; $k_2 = 0.03$ d$^{-1}$ with $t_\text{½} = 23.5$ d, contaminated water + 4% ration uncontaminated food,

$k_1 = 0.265$ d$^{-1}$; $k_2 = 0.037$ d$^{-1}$ with $t_\text{½} = 18.7$ d, uncontaminated water + 8% ration contaminated food,

$k_1 = 185.5$ d$^{-1}$; $k_2 = 0.027$ d$^{-1}$ with $t_\text{½} = 25.5$ d, contaminated water + 8% ration uncontaminated food,

$k_1 = 0.262$ d$^{-1}$; $k_2 = 0.032$ d$^{-1}$ with $t_\text{½} = 21.5$ d, contaminated food (4% ration) then water,

$k_1 = 214$ d$^{-1}$; $k_2 = 0.023$ d$^{-1}$ with $t_\text{½} = 29.9$ d, contaminated water then food (4% ration)

$k_1 = 0.292$ d$^{-1}$; $k_2 = 0.043$ d$^{-1}$ with $t_\text{½} = 16.2$ d, contaminated food (8% ration) then water,

$k_1 = 154$ d$^{-1}$; $k_2 = 0.020$ d$^{-1}$ with $t_\text{½} = 35.4$ d, contaminated water then food (8% ration)

Kinetic data of grass shrimps in 16-d uptake and 21-d clearance studies (Fisher & Clark 1990)

$k_1 = 0.475$ d$^{-1}$; $k_2 = 0.017$ d$^{-1}$ with $t_\text{½} = 28$ d, uncontaminated water + 4% ration contaminated food,

$k_1 = 175$ d$^{-1}$; $k_2 = 0.014$ d$^{-1}$ with $t_\text{½} = 47.8$ d, contaminated water + 4% ration uncontaminated food,

$k_1 = 0.499$ d$^{-1}$; $k_2 = 0.019$ d$^{-1}$ with $t_\text{½} = 36.3$ d, contaminated food (4% ration) then water,

$k_1 = 182$ d$^{-1}$; $k_2 = 0.013$ d$^{-1}$ with $t_\text{½} = 51.5$ d, contaminated water then food (4% ration)

$k_1 = 0.399$ d$^{-1}$; $k_2 = 0.021$ d$^{-1}$ with $t_\text{½} = 32.3$ d, contaminated food (8% ration) then water,

$k_1 = 170$ d$^{-1}$; $k_2 = 0.011$ d$^{-1}$ with $t_\text{½} = 63.7$ d, contaminated water then food (4% ration)

Half-Lives in the Environment:

Air: estimated $t_\text{½} = 438,000$ to $4.2 \times 10^7$ h or 50–200 yr (Howard et al. 1991).

Surface water: $t_\text{½} = 7488$ to 17,280 h or 312 d to 2 yr, based on aerobic aquatic microcosm study (Howard et al. 1991).

Ground water: estimated $t_\text{½} = 14,976$ to 34,560 h (624 d to 4 yr) based on aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: estimated $t_\text{½} = 14,976$ to 34,560 h (624 d to 4 yr) based on aerobic aquatic microcosm study (Howard et al. 1991).

Biota: clearance $t_\text{½} = 28$ d (shrimp, 10–20 d exposure, Bahner 1977)

Clearance $t_\text{½} = 16.2–35.4$ d for spot Leiostomus xanthurus (Fisher et al. 1986):

$t_\text{½}(4W) = 18.7$ d for kepone contaminated water + uncontaminated food at 4% ration

$t_\text{½}(4F) = 23.5$ d for uncontaminated water + kepone contaminated food at 4% ration
t₁/₂(8W) = 18.7 d for kepone contaminated water + uncontaminated food at 8% ration,

\[ t₁/₂(8F) = 25.5 \text{ d} \text{ for uncontaminated water + kepone contaminated food at 8\% ration} \]

\[ t₁/₂(4FW-food) = 21.5 \text{ d} \text{ for dietary accumulation in combined exposure (food-water) at 4\% ration} \]

\[ t₁/₂(4FW-water) = 29.9 \text{ d} \text{ for dietary accumulation in combined exposure (water-food) at 4\% ration} \]

\[ t₁/₂(8FW-food) = 16.2 \text{ d} \text{ for dietary accumulation in combined exposure (food-water) at 8\% ration} \]

\[ t₁/₂(8FW-water) = 35.4 \text{ d} \text{ for dietary accumulation in combined exposure (water-food) at 8\% ration} \]

Clearance \[ tᵦ = 32.3–63.7 \text{ d} \text{ for grass shrimps } Palaemonetes pugio \text{ (Fisher & Clark 1990):} \]

\[ tᵦ(4W) = 47.8 \text{ d} \text{ for kepone contaminated water + uncontaminated food at 4\% ration} \]

\[ tᵦ(4F) = 40.6 \text{ d} \text{ for uncontaminated water + kepone contaminated food at 4\% ration} \]

\[ tᵦ(4FW-food) = 36.3 \text{ d} \text{ for dietary accumulation in combined exposure (food-water) at 4\% ration} \]

\[ tᵦ(4FW-water) = 51.5 \text{ d} \text{ for dietary accumulation in combined exposure (water-food) at 4\% ration} \]

\[ tᵦ(8FW-food) = 32.3 \text{ d} \text{ for dietary accumulation in combined exposure (food-water) at 8\% ration} \]

\[ tᵦ(8FW-water) = 63.7 \text{ d} \text{ for dietary accumulation in combined exposure (water-food) at 8\% ration} \]
18.1.1.53 Leptophos

Common Name: Leptophos
Synonym: Abar, Phosvel, VCS-506
Chemical Name: \( \text{O-(4-bromo-2,5-dichlorophenyl) O-methyl phenylphosphorothioate} \)
Uses: insecticide
CAS Registry No: 21609-90-5
Molecular Formula: \( \text{C}_{13}\text{H}_{10}\text{BrCl}_{2}\text{O}_{2}\text{PS} \)
Molecular Weight: 412.066
Melting Point (°C):
71 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
1.53 (25°C, Merck Index 1989)
Molar Volume (cm\(^3\)/mol):
317.8 (calculated-Le Bas method at normal boiling point)
269.3 (calculated-density)
Dissociation Constant, \( pK_a \):
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), \( F \): 0.354 (mp at 71°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
0.03 (shake flask-UV, Carringer et al. 1975)
0.03 (20°C, GC, Freed 1976)
0.0047 (20°C, shake flask-GC, Chiou et al. 1977)
2.4 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980)
0.07 (20°C, shake flask-GC, Bowman & Sans 1979)
0.0047 (20–25°C, shake flask-GC, Freed et al. 1979)
0.005 (20–25°C, shake flask-GC, Kanazawa 1981)
0.021 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
0.03 (Budavari 1989)
Vapor Pressure (Pa at 25°C or as indicated):
\( 3.07 \times 10^{-6} \) (20°C, NIEHS 1975; quoted, Freed et al. 1977)
\( 2.27 \times 10^{-5} \) (30°C, NIEHS 1975; quoted, Freed et al. 1977)
\( 3.07 \times 10^{-6} \) (20–25°C, Freed et al. 1979)
\( 3.00 \times 10^{-6} \) (20°C, selected, Suntio et al. 1988)
0.0002 (Merck Index 1989)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
0.27 (20°C, calculated-P/C, Mackay & Shiu 1981)
0.25 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
6.30 (NIEHS 1975; quoted, Freed et al. 1977)
6.31 (20°C, shake flask-GC, Chiou et al. 1977)
6.31 (Hansch & Leo 1979)
4.32 (20°C, shake flask-GC, Kanazawa 1981)
Insecticides

5.88  (22°C, shake flask-GC, Bowman & Sans 1983b)
6.31  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.81   *(Daphnia magna*, wet wt. basis, Macek et al. 1979)
2.88, 3.16  (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
2.58, 2.86  (calculated-S, calculated-*K*_{OEC}, Kenaga 1980)
3.78   *(Pseudorasbora parva*, Kanazawa 1981)
3.16   (mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
3.78   (topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
2.88   (fish, reported as log BAF_{W}, LeBlanc 1995)

Sorption Partition Coefficient, log *K*_{OC}:
3.97   (soil, Carringer et al. 1975)
3.43   (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.97, 4.45  (reported as log *K*_{OM}, estimated as log *K*_{OM}, Magee 1991)
4.50   (soil, calculated-MCI 1 χ, Sabljic et al. 1995)
3.88, 4.74  (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, *t*_{1/2}:

Half-Lives in the Environment:
Common Name: Lindane (γ-HCH)
Chemical Name: 1,2,3,4,5,6-hexachlorocyclohexane; γ-hexachlorocyclohexane; γ-1,2,3,4,5,6-hexachloro-cyclohexane; 1α,2α,3β,4α,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane
Uses: insecticide and pesticide with contact, stomach, and respiratory action to control a broad spectrum of phytophagous and soil inhibiting insects, public health pests, and animal ectoparasites.
CAS Registry No: 58-89-9
Molecular Formula: C6H6Cl6
Molecular Weight: 290.830
Melting Point (°C):
112.5 (Slade 1945; Howard 1991; Montgomery 1993; Milne 1995; Lide 2003)
Boiling Point (°C):
323.4 (Howard 1991; Montgomery 1993; Lide 2003)
Density (g/cm³ at 20°C):
1.87 (Montgomery 1993)
Molar Volume (cm³/mol):
243.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHv (kJ/mol):
101.13 (Spencer & Cliath 1970)
76 (Rordorf 1989)
Enthalpy of Fusion, ΔHfus (kJ/mol):
22.4 (Rordorf 1989)
22.13 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔSfus (J/mol K):
41.4 (Plato & Glasgow 1969)
58.0 (Rordorf 1989)
61.1 (Hinckley et al. 1990; Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
0.12 (20°C, Suntio et al. 1988)
0.138 (Mackay et al. 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):
10 (20°C, Slade 1945; Günther et al. 1968; Spencer 1973, 1982)
7.3* (shake flask-UV spectrophotometry, measured range 25–45°C, Richardson & Miller 1960)
0.50–6.60 (particle size of 0.04–5μ, shake flask-GC, room temp., Robeck et al. 1965)
5.7 (partition coefficient, Atkins & Eggleton 1971)
7.52 ± 0.041 (shake flask-centrifuge/GC, Masterton & Lee 1972)
7.40, 5.75 (28°C, shake flask-centrifuge, membrane filter-GC, maximum 0.1 µm particle size, Kurihara et al. 1973)
6.61, 6.24 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 µm particle size, Kurihara et al. 1973)
12 (26.5°C, Bhavnagary & Jayaram 1974)
0.15*, 0.60*, 6.80* (shake flask-GC, for different particle sizes: 0.01µ, 0.05µ, 5.0µ, measured range 15–45°C, Biggar & Riggs 1974)
7.8 (generator column-GC/ECD, Weil et al. 1974)
0.15 (Martin & Worthing 1977; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
2.0 (shake flask-nephelometry, Hollifield 1979)
10.3 (shake flask-GC/ECD, Malaiyandi et al. 1982)
9.50, 7.9–8.2 (shake flask-GC/ECD: Milli-Q water, environmental surface waters, Saleh et al. 1982)
6.11 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991; 1993)
7.87 (24°C, shake flask-GC, Chiu et al. 1986)
7.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
log [S_i/(mol/L)] = 2.220 – 1237/(T/K) (liquid, Passivirta et al. 1999)
67.77, 71.84 (supercooled liquid S_i: derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)
log [S_i/(mol m⁻³)] = −749.8/(T/K) + 2.78 (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
log [S_i/(mol m⁻³)] = −788.4/(T/K) + 2.04 (supercooled liquid, final adjusted eq., Xiao 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):
4.0, 18.7, 64(20, 40, 60°C static method, Slade 1945)
0.001253* (20°C, effusion manometer, measured range 0–90°C, Balson 1947)
log (P/mmHg) = 15.515 – 6020/(T/K); temp range 50–90°C, (effusion manometer, Balson 1947)
0.00435* (20°C, gas-saturation-GC, measured range 20–40°C, Spencer & Cliath 1970)
log (P/mmHg) = 13.544 – 5288/(T/K), temp range 20–40°C (gas saturation-GC, Spencer & Cliath 1970)
0.00413 (20°C, Partition coefficient, Atkins & Eggleton 1971)
0.0213 (20°C, Demozay & Marechal 1972)
0.00125 (20°C, Martin 1972, Melnikov 1971, Spencer 1973; Montgomery 1993)
0.0028 (20°C, estimated from diffusion rate, Zimmerli & Marek 1974)
0.0026 (20°C, estimated-relative loss rate, Dobbs & Grant 1980)
0.00426 (20°C, volatilization rate, Burkhard & Guth 1981)
log (P/mmHg) = 15.515 – 6020/(T/K) (Gückel et al. 1982)
0.166 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.107, 0.0654 (Pₚc by GC-RT correlation, different stationary phases, Bidleman 1984)
0.0552 (supercooled liquid Pₚc, converted from literature Pₛ with ∆Sₙₛ Bidleman 1984)
0.00321; 0.00368 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
0.00435 (20°C, GC-RT correlation, Kim 1985)
6.70 × 10⁻⁸ (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
log (Pₚ/Pₚc) = 15.096 – 5148.9/(T/K); measured range 45–113°C (solid, gas saturation-GC, Rordorf 1989)
log (Pₚ/Pₚc) = 12.05 – 3970.1/(T/K); measured range 115–171°C (liquid, gas saturation-GC, Rordorf 1989)
0.0552, 0.0649 (supercooled Pₚc, converted from literature Pₛ with different ∆Sₙₛ values, Hinckley et al. 1990)
0.107, 0.0706 (Pₚc by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (Pₚ/Pₚc) = 11.15 – 3680/(T/K) (GC-RT correlation, supercooled liquid Pₚc, Hinckley et al. 1990; quoted, Boehncke et al. 1996))
7.426 × 10⁻⁴ (Howard 1991)
0.0044 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0145, 0.0398, 0.1035 (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bildeman 1992)

0.0094* (20°C, gas saturation-GC/ECD, measured range –30 to 30°C, Wania et al. 1994; quoted, Boehncke et al. 1996)

\[ \log(P/Pa) = 16.99 - 5566/(T/K) \], temp range –30 to +30°C (solid, gas saturation-GC, Wania et al. 1994)

0.00737* (Knudsen effusion method, measured range 19.63–53.07°C, Boehncke et al. 1996)

0.00383 (20°C, interpolated from vapor pressure eq. \( \ln(P/Pa) = (34.53 \pm 0.21) - (11754 \pm 72)/(T/K) \), temp range 20–50°C, Boehncke et al. 1996)

0.0104* (torsion and Knudsen-effusion methods, measured range 310–384 K, Giustini et al. 1998)

\[ \log(P/kPa) = (11.23 \pm 0.50) - (4832 \pm 150)/(T/K) \], temp range 310–384 K (torsion and Knudsen-effusion methods, Giustini et al. 1998)

0.189, 0.131; 0.0167 (quoted supercooled liquid \( P_L \): calculated, GC-RT correlation; converted to solid \( P_S \) with fugacity ratio \( F \), Passivirta et al. 1999)

\[ \log(P_L/Pa) = 13.80 - 4330/(T/K) \], (supercooled liquid, Passivirta et al. 1999)

0.0776, 0.0759 (supercooled liquid \( P_L \): LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)

\[ \log(P/Pa) = -3890/(T/K) + 11.94 \] (supercooled liquid, linear regression of literature data, Xiao et al. 2004)

\[ \log(P/Pa) = -3905/(T/K) + 11.98 \] (supercooled liquid, final adjusted eq., Xiao et al. 2004)

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

0.005 (calculated-P/C, Mackay & Leinonen 1975)

0.22 (gas stripping, Atkins & Eggleton 1971)

0.32 (24°C, calculated-P/C, Chiou et al. 1980)

0.018–0.55 (calculated-P/C, Mabey et al. 1982)

0.124 (20°C, volatilization rate, Burkhard & Guth 1981)

0.27–0.32 (calculated-P/C, Mackay & Shiu 1981)

0.05 (calculated-P/C, Lyman et al. 1982; quoted, Suntio et al. 1988)

0.0486 (calculated-P/C, Thomas 1982)

0.322 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)

0.158 (calculated-P/C, Mackay et al. 1986)

0.202, 0.234 (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)

1.49 (WERL Treatability Database, Ryan et al. 1988)

0.129 (20°C, calculated-P/C, Suntio et al. 1988)

0.322 (calculated-P/C, Taylor & Glotfelty 1988)

0.199, 0.209 (22–24°C, fog chamber-concentration ratio-GC/ECD, Fendinger et al. 1989)

0.0486 (20°C, Lyman et al. 1990; quoted, Hemond & Fechner 1994)

0.10 (calculated-P/C, Ballshmiter & Wittlinger 1991; Fischer et al. 1991)

0.296 (calculated-P/C, Howard 1991)

0.353* (distilled water, gas stripping-GC/ECD, measured range 0.5–45°C, Kucklick et al. 1991)

\[ \log[H/(Pa·m³ mol⁻¹)] = -2382/(T/K) + 7.54 \], temp range: 0.5–45°C (gas stripping-GC/ECD, Kucklick et al. 1991, McConnell et al. 1993)

0.0627, 0.137, 0.363, 0.996, 2.57 (0.5, 10, 23, 35, 45°C, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

\[ \log[H/(Pa·m³ mol⁻¹)] = -2703/(T/K) + 8.68 \] (gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

\[ \log[H/(Pa·m³ mol⁻¹)] = -2703/(T/K) + 8.68 \] (gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

0.17 (calculated-P/C, Calamari et al. 1991)

0.10, 1.50 (calculated-P/C, Fischer et al. 1991)

25.9 (calculated-bond contribution method, Meylan & Howard 1991)

0.13 (20°C), 0.20, 0.339, 0.363 (23°C), 0.158 (Iwata et al. 1993)

0.121 at 8°C in Green Bay, 0.242 at 18.9°C in Lake Michigan, 0.236 at 18.5°C in Lake Huron, 0.301 at 22.3°C in Lake Erie and 0.301 at 22.3°C in Lake Ontario (concn ratio-GC, McConnell et al. 1993)

0.0246 (20°C, Montgomery 1993)

0.520 (wetted wall column-GC, Altschuh et al. 1999)

\[ \log[H/(Pa·m³ mol⁻¹)] = 11.58 – 3049/(T/K) \] (Passivirta et al. 1999)

0.18* (20°C, air stripping-GC, measured range 10–40°C, Jantunen et al. 2000)
Insecticides

\[
\log \left[ \frac{[H]}{(Pa \ m^3/mol)} \right] = 9.51 - 3005/(T/K); \text{ temp range 10–40°C (gas stripping, Jantunen et al. 2000)}
\]
\[
0.258 \quad \text{(20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)}
\]
\[
\log K_{AW} = 3.715 - 2254/(T/K); \text{ temp range 10–40°C (gas stripping, van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)}
\]
\[
0.14^* \quad \text{(20°C, dynamic headspace-GC, DHS method, measured range 5–35°C, Sahsuvar et al. 2003)}
\]
\[
0.15^* \quad \text{(20°C, gas stripping-GC, BS method, measured range 5–35°C, Sahsuvar et al. 2003)}
\]
\[
0.14^* \quad \text{(20°C, mean value of DHS and BS methods, temp range 5–35°C, Sahsuvar et al. 2003)}
\]
\[
\log \left[ \frac{[H]}{(Pa \ m^3/mol)} \right] = 10.14 - 3208/(T/K); \text{ temp range 5–35°C (Sahsuvar et al. 2003)}
\]
\[
0.159, 0.193 \quad \text{(20, 23°C, dynamic equilibrium system-GC/MS, measured range 278–293 K, Feigenbrugel et al. 2004)}
\]
\[
0.269, 0.309 \quad \text{(LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)}
\]
\[
\log \left[ \frac{[H]}{(Pa \ m^3/mol)} \right] = -2940/(T/K) + 9.29 \quad \text{(LDV linear regression of literature data, Xiao et al. 2004)}
\]
\[
\log \left[ \frac{[H]}{(Pa \ m^3/mol)} \right] = -3117/(T/K) + 9.94 \quad \text{(FAV final adjusted eq., Xiao et al. 2004)}
\]
\[
0.165^* \quad \text{(seawater, dynamic equilibrium system-GC/MS, measured range 278–293 K, Xiao et al. 2004)}
\]

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

3.72 \quad \text{(shake flask-GC, Kurihara et al. 1973)}
3.65 \quad \text{(HPLC-RT correlation, Sugiura et al. 1979)}
3.85 \quad \text{(HPLC-RT correlation, Veith et al. 1979)}
2.81 \quad \text{(Rao & Davidson 1980)}
3.66 \quad \text{(shake flask-GC, conc. ratio, Kanazawa 1981)}
3.62 \quad \text{(HPLC-k' correlation, McDuffie 1981)}
3.25 \quad \text{(shake flask-GC, Platford 1982)}
3.53 \quad \text{(shake flask-GC/FID, Hermens & Leeuwangh 1982)}
3.90 \quad \text{(Elgar 1983)}
3.61 \quad \text{(Hansch & Leo 1985)}
3.67 \quad \text{(HPLC-RT correlation, Eadsforth 1986)}
3.00 \quad \text{(HPLC-RT correlation, De Kock & Lord 1987)}
3.57 \quad \text{(shake flask-GC, Kishi & Hashimoto 1989)}
3.688 \pm 0.021 \quad \text{(shake flask/slow stirring-GC, De Bruijn et al. 1989)}
3.51 \quad \text{(shake flask-GC, Noegrohati & Hammers 1992)}
3.20–3.89 \quad \text{(Montgomery 1993)}
5.32 \quad \text{(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)}
3.55 \quad \text{(recommended, Sangster 1993)}
3.52 \quad \text{(RP-HPLC-RT correlation, Finizio et al. 1997)}
3.72^* \pm 0.01 \quad \text{(shake flask-slow stirring-GC, measured range 5–35°C, Paschke & Schüermann 1998)}
3.80; 3.71 \quad \text{(quoted lit.; calculated, Passivirta et al. 1999)}
3.70, 3.83 \quad \text{(LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)}
\log K_{OW} = 282.2/(T/K) + 2.78 \quad \text{(LDV linear regression of literature data, Xiao et al. 2004)}
\log K_{OW} = 533.2/(T/K) + 2.04 \quad \text{(LDV linear regression of literature data, Xiao et al. 2004)}

Octanol/Air Partition Coefficient, \(K_{OA}\) at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *
* are compiled at the end of this section:

7.70 \quad \text{(calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)}
8.08 \quad \text{(calculated, Finizio et al. 1997)}
7.847^*, 7.849 \quad \text{(gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)}
\log K_{OA} = -3.61 + 3415/(T/K); \text{ temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)}
7.84, 7.74 \quad \text{(LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)}
\log K_{OA} = 3415/(T/K) - 3.61 \quad \text{(LDV linear regression of literature data, Xiao et al. 2004)}
\log K_{OA} = 3521/(T/K) - 4.07 \quad \text{(FAV final adjusted eq., Xiao et al. 2004)}

Bioconcentration Factor, \(B_{cm}\), log BCF:

\[-1.78 \quad \text{(beef biotransfer factor log } B_{cm}, \text{ correlated-K_{OW}, Radeleff et al. 1952; Kenaga 1980;\)}\]
\[-0.41 \quad \text{(vegetation, correlated-K_{OW}, Lichtenstein 1959; Voerman & Besemer 1975)}\]
\[-2.60 \quad \text{(milk biotransfer factor log } B_{cm}, \text{ correlated-K_{OW}, Saha 1969)\)}\]
2.15, 2.34 (Voerman & Tammes 1969)
1.83, 3.24 (brine shrimp, silverside fish, Matsumura & Benezet 1973)
1.98, 2.26 (brine shrimp in water, brine shrimp in sand, Matsumura & Benezet 1973)
3.21 (northern brook silverside fish to lindane residues on sand, Matsumura & Benezet 1973)
2.75, 2.66 (fish, snail, Metcalf et al. 1973)
2.26 (fathead minnow, Canton et al. 1975)
2.23, 2.65 (zooplankton, Hamelink & Waybrant 1976)
2.00 (mussels, steady state, Ernst 1977)
1.92, 2.34, 1.80, 2.69 (pink shrimp, pinfish, grass shrimp, sheepshead minnow, Schimmel et al. 1977; quoted, Howard 1991)
2.88, 2.45, 2.65, 2.97 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
2.68 (fathead minnow, Veith et al. 1979)
2.26 (fathead minnow, 32-d exposure, Veith et al. 1979; Veith & Kosian 1983)
2.51, 2.75 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
3.26, 1.73 (calculated-S, KOC, Kenaga 1980)
–0.26 (average beef fat diet, Kenaga 1980b)
2.67, 2.25 (fathead minnow, 32-d exposure, Veith et al. 1980)
3.10 (topmouth gudgeon, Kanazawa 1981)
2.19 (mussel, quoted average, Geyer et al. 1982)
3.10 (topmouth gudgeon, Kanazawa 1983)
3.42 (clam fat, 60-d exptl., Hartley & Johnson 1983)
2.38, 2.46 (algae: exptl., calculated, Geyer et al. 1984)
2.26 (fathead minnow, Davies & Dobbs 1984)
2.38, 2.88, 2.91 (algae, fish, activated sludge, Klein et al. 1984)
2.38, 2.57, 2.91 (algae, golden ide, activated sludge, Freitag et al. 1985)
2.89–3.32 mean 3.08; 2.94–5.46 mean 3.30 (p,p′-DDT, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
3.32, 3.20; 3.00 (rainbow trout: kinetic BCF, steady-state BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
2.50 (Salmo gairdneri Richardson fry, Ramamooorthy 1985)
2.78, 2.73, 2.78, 2.61 (mussel, pinfish, sheepshead minnow; calculated-Kow and models, Zaroogian et al. 1985)
2.38, 2.67 (quoted values: mussel, sheepshead minnow, Zaroogian et al. 1985)
2.76; 2.43 (salmon fry in humic water April 1982; Oct. 1983, at steady state, Carberg et al. 1986)
2.42, 2.84; 2.45–3.18 (salmon fry in lake water, quoted lit. values, Carberg et al. 1986)
2.33 (Daphnia magna, wet wt. basis, Korte & Freitag 1986)
3.53 (azalea leaves, Bacci & Gaggi 1987)
2.38 (paddy field fish, Soon & Hock 1987)
4.30 (zooplankton, chum salmon, Kawano et al. 1988)
3.53, 5.88 (dry leaf, wet leaf, Bacci et al. 1990)
2.33 (Daphnia magna, Geyer et al. 1991)
2.09, 2.70, 2.29, 2.34 (zebrafish: egg, embryo, yolk sac fry, juvenile, Gorge & Nagel 1990)
1.96 (calculated, Banerjee & Baughman 1991)
2.93, 2.96 (Brachydanius reri, Butte et al. 1991)
2.67 (selected, Chesebsells et al. 1992)
1.58 (Hydridil, Hinman & Klaine 1992)
2.16–2.57 (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992; quoted, Devillers et al. 1996)
3.77–3.85 (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)
2.65 ± 2.23; 1.63–3.63 (aquatic organisms, wet wt basis, average value; range, Geyer et al. 1997)
4.04 (aquatic organisms, lipid basis, Geyer et al. 1997)
2.65; 2.606, 2.676 (fish, steady-state, quoted lit.; calculated-MCI χ, calculated-Kow Lu et al.1999)

Sorption Partition Coefficient, log KOC:
2.96 (soil, Hamaker & Thompson 1972; Kenaga 1980a, b; Kenaga & Goring 1980)
4.09 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.40 (soil, Kenaga 1980)
2.87 (average of 3 soils, HPLC-RT, McCall et al. 1980)
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization: $t_{1/2} = 191 \text{ d}$ was estimated from water (Mackay & Leinonen 1975, quoted, Howard 1991)
- estimated $t_{1/2} > 200 \text{ d}$ (Callahan et al. 1979);
- $t_{1/2} (\text{exptl.}) = 3.2 \text{ d}$ in nonstirred water and $t_{1/2} (\text{exptl.}) = 1.5 \text{ d}$ in stirred water from 4.5 cm deep distilled water at $24^\circ\text{C}$ (Chiou et al. 1980; quoted, Howard 1991);
- estimated half-lives: 3.4 d in nonstirred water and 2.3 d in stirred water (Chiou et al. 1980);
- $t_{1/2} = 22 \text{ d}$, estimated from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);
- initial $k = 4.4 \times 10^{-2} \text{ h}^{-1}$ and predicted $k = 1.4 \times 10^{-2} \text{ h}^{-1}$ from soil with $t_{1/2} = 49.5 \text{ h}$ (Thomas 1982);
- $t_{1/2} (\text{calc}) = 2760 \text{ h}$ from water (Thomas 1982);
- measured rate constant $k(\text{exptl.}) = 3.0 \text{ d}^{-1}$ (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989);
- calculated rate constant $k = 0.01 \text{ d}^{-1}$ (Glotfelty et al. 1989);
- $t_{1/2} = 266 \text{ d}$ from lab. and field experiments (Jury et al. 1984; quoted, Spencer & Cliaith 1990);
- half-lives in soil surfaces at $20 \pm 1^\circ\text{C}$: $t_{1/2} = 5.5$ to 15.9 d in peat soil and $t_{1/2} = 2.7$ to 6.7 d in sandy soil;
- half-lives in plant surfaces at $20 \pm 1^\circ\text{C}$: $t_{1/2} = 0.56 \text{ d}$ in bean, $t_{1/2} = 0.40 \text{ d}$ in turnips and $t_{1/2} = 0.31 \text{ d}$ in oats (Dörfler et al. 1991).

Photolysis: $k_p(\text{aq.}) = 1.429 \times 10^{-2} \text{ d}^{-1}$ for photolysis in natural waters (Malaiyandi et al. 1982)
- $k_p(\text{aq.}) = 8.9 \times 10^{-4} \text{ h}^{-1}$ for Milli-Q water, $k_p = 4.1 \times 10^{-3} \text{ h}^{-1}$ for natural surface water samples from eutrophic pond, $k_p = 3.9 \times 10^{-3} \text{ h}^{-1}$ from eutrophic pond, $k_p = 4.5 \times 10^{-4} \text{ h}^{-1}$ from oligotrophic rock quarry and the half-lives were 779, 169, 1791, and 1540 h, respectively, under direct sunlight (Saleh et al. 1982; quoted, Howard 1991).

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:
- $k_{OH} = 6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a $t_{1/2} \approx 2.3 \text{ d}$ (Atkinson 1987; quoted, Howard 1991)
- $k(\text{aq.}) = 4.2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to DBCP) with hydroxyl radical in aqueous solutions at pH 2.9 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoenig 1990; Haag & Yao 1992)
- $k(\text{aq.}) \leq 0.04 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.3 and 23°C, with a $t_{1/2} \geq 10 \text{ d}$ at pH 7 (Yao & Haag 1991).
calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992).

\[ k_{OH}(aq.) = (5.8 \pm 1.9) \times 10^8 \text{ M}^{-1} \text{s}^{-1} \] (Fenton with reference to DBCP); and \( k = (5.2 \pm 0.9) \times 10^8 \text{ M}^{-1} \text{s}^{-1} \) (photo-Fenton with reference to DBCP) for the reaction with hydroxyl radicals in aqueous solutions at pH 2.9 and at 24 ± 1°C (Haag & Yao 1992)

**Hydrolysis:** \( k(\text{neutral}) = 1.6 \times 10^{-4} \text{ h}^{-1} \) indicating that neutral hydrolysis is unimportant, rate constants of 7.5 × 10⁻³, 8.99 × 10⁻⁴, and 1.07 × 10⁻³ h⁻¹ corresponded to half-lives of 92, 771 and 648 h in natural surface water samples from eutrophic pond, dystrophic reservoir and oligotrophic rock quarry, respectively (Saleh et al. 1982; quoted, Howard 1991).

\[ k(\text{neutral}) = (1.2 \pm 0.2) \times 10^{-4} \text{ h}^{-1} \] with a calculated \( t_{1/2} = 206 \text{ d} \) at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993).

\[ t_{1/2} = 42 \text{ yr at pH 8 and 5°C} \] (Ngabe et al. 1993).

\[ t_{1/2} = 191 \text{ d at pH 7, and } t_{1/2} = 11 \text{ h at pH 9 at 22°C} \] (Tomlin 1994).

\[ t_{1/2} = 240 \text{ d at pH 2, } t_{1/2} = 210 \text{ d at pH 7 and } t_{1/2} = 0.015 \text{ d at pH 12 in natural waters} \] (Capel & Larson 1995).

**Biodegradation:** \( k = 0.0026 \text{ d}^{-1} \) by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982).

\[ t_{1/2} = \text{half-life of } 266 \text{ d (soil, Jury et al. 1987); } t_{1/2} = \text{3 to 30, 30 to 300 d and >300 d for river, lake and ground water, respectively} \] (Zoeteman et al. 1980; quoted, Howard 1991).

\[ t_{1/2} = 266 \text{ d for 100-d leaching screening test in } 0–10 \text{ cm depth of soil} \] (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989).

\[ t_{1/2}(\text{aerobic}) = 31 \text{ d, } t_{1/2}(\text{anaerobic}) = 5.9 \text{ d in natural waters} \] (Capel & Larson 1995).

\[ t_{1/2}(\text{calc}) = (20.4 \pm 0.1) \text{ h in sewage sludge from experiments S1–S3} \] (Buser & Müller 1995).

**Biotransformation:**

**Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[ k_1 = 3.13 \text{ h}^{-1}; k_2 = 0.0313 \text{ h}^{-1} \] (mussels, Ernst 1977)

\[ k_1 = 130 \text{ d}^{-1}; k_2 = 0.063 \text{ d}^{-1} \] (rainbow trout, Oliver & Niimi 1985)

\[ k_1 = 14, 179, 196 \text{ h}^{-1} \] (zebrafish: egg, yolk sac fry, juvenile, Görgé & Nagel 1990)

\[ k_1 = 0.06 \text{ h}^{-1} \] (Chironomus riparius-water only system, Lydy et al. 1992)

\[ k_1 = 0.0661 \text{ h}^{-1} \] (Chironomus riparius-screened system, Lydy et al. 1992)

\[ k_1 = 0.08 \text{ h}^{-1} \] (Chironomus riparius-3% organic carbon system, Lydy et al. 1992)

\[ k_1 = 0.0661 \text{ h}^{-1} \] (Chironomus riparius-15% organic carbon system, Lydy et al. 1992)

\[ k_1 = 9.0–26.4 \text{ h}^{-1}; k_2 = 0.04–0.18 \text{ h}^{-1} \] (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992)

\[ k_1 = 180–939 \text{ h}^{-1}; k_2 = 0.031–0.13 \text{ h}^{-1} \] (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)

**Half-Lives in the Environment:**

**Air:** \( t_{1/2} \sim 2.3 \text{ d} \) was estimated, based on rate constant \( 6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{s}^{-1} \) for the vapor-phase reaction with hydroxyl radical in air (Howard 1991); calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992); atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).

Lifetime of 13 d was estimated for atmospheric reaction with OH radical in the tropics (Schreitmüller and Ballschmitter 1995); halflives in the Great Lake’s atmosphere. \( t_{1/2} = 7.9 \pm 1.2 \text{ yr at Eagle Harbor, } t_{1/2} = 4.3 \pm 0.5 \text{ yr at Sleeping Bear Dunes and } t_{1/2} = 4.9 \pm 0.5 \text{ yr at Sturgeon Point, when accounting the agricultural application effects, half-lives are, } t_{1/2} = 9.1 \pm 1.3 \text{ yr at Eagle Harbor, } t_{1/2} = 4.6 \pm 0.4 \text{ yr at Sleeping Bear Dunes and } t_{1/2} = 5.4 \pm 0.4 \text{ yr at Sturgeon Point} \) (Buehler et al. 2004).

**Surface water:** \( t_{1/2} = 10–138 \text{ d} \) in various locations in the Netherlands in case a first order reduction process may be assumed; and \( t_{1/2} = 3–30 \text{ d in rivers and } t_{1/2} = 30–300 \text{ d in lakes} \) (Zoeteman et al. 1980).

hydrolysis \( t_{1/2}(\text{exptl}) = 92 \text{ h, } t_{1/2}(\text{calc}) = 89 \text{ h} \) for Roselawn Cemetery Pond at pH 9.3; \( t_{1/2}(\text{exptl}) = 771 \text{ h, } t_{1/2}(\text{calc}) = 578 \text{ h} \) for Cross Lake at pH 7.3; \( t_{1/2}(\text{exptl}) = 648 \text{ h, } t_{1/2}(\text{calc}) = 231 \text{ h} \) for Indiana Quarry at pH 7.8; photolysis half-lives for direct sunlight during July and adjusted for mid-winter: \( t_{1/2} = 779 \text{ h, } 1560 \text{ h} \) for Milli-Q water at pH 6.98, \( t_{1/2} = 169 \text{ h, } 339 \text{ h} \) for Roselawn Pond at pH 9.3, \( t_{1/2} = 1791 \text{ h, } 3590 \text{ h} \) for Cross Lake and \( t_{1/2} = 1540 \text{ h, } 3090 \text{ h} \) for Indiana Quarry (Saleh et al. 1982).

\( t_{1/2} > 10 \text{ d} \) for direction reaction with ozone in water at 23°C and pH 7 (Yao & Haag 1991);
hydrolysis $t_{1/2} = 191 \text{ d at pH 7, and } t_{1/2} = 11 \text{ h at pH 9 at } 22^\circ \text{C (Tomlin 1994).}$
Biodegradation $t_{1/2}^{\text{(aerobic)}} = 31 \text{ d, } t_{1/2}^{\text{(anaerobic)}} = 5.9 \text{ d, hydrolysis } t_{1/2} = 240 \text{ d at pH 2, } t_{1/2} = 210 \text{ d at pH 7}$
and $t_{1/2} = 0.015 \text{ d at pH 12 in natural waters (Capel & Larson 1995).}$

Ground water: $t_{1/2} = 300 \text{ d (Zoeteman et al. 1980).}$

Sediment:
Soil: $t_{1/2} = 2 \text{ yr persistence in soil (Nash & Woolson 1967; quoted, Kaufman 1976);}$
persistence of 3 yr in soil (Edwards 1973; quoted, Morrill et al. 1982);
t $t_{1/2} > 50 \text{ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988)}$
First-order $t_{1/2} = 266 \text{ d in soil from biodegradation rate constant } k = 0.0026 \text{ d}^{-1}$ by die-away test in soil
(Rao & Davidson 1980; quoted, Scow 1982);
field $t_{1/2} = 0.3 \text{ d in moist fallow soil (Glotfelty 1981; quoted, Nash 1983);}$
macroagroecosystem $t_{1/2} = 1-4 \text{ d in moist fallow soil (Nash 1983); measured dissipation rate of } 0.16 \text{ d}^{-1}$ (Nash 1983; quoted, Nash 1988);
estimated dissipation rate of 0.20, 0.10 $\text{d}^{-1}$ (Nash 1988);
biodegradation $t_{1/2} = 266 \text{ d (soil, Jury et al. 1984, 1987);}$
first-order adsorption rate 0.088 $\text{h}^{-1}$ (Miller & Weber 1986; quoted, Brusseau & Rao 1989);
half-lives in soil surfaces at 20 ± 1°C: $t_{1/2} = 5.5$ to 15.9 d in peat soil and $t_{1/2} = 2.7$ to 6.7 d in sandy soil
(Dörfler et al. 1991); reported $t_{1/2} = 266 \text{ d in soil (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted,}$
Montgomery 1993);
reaction $t_{1/2} = 266 \text{ d (Mackay & Stiver 1991);}$
selected field $t_{1/2} = 400 \text{ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);}$
$5.5$ to 15.9 d in peat soil and $t_{1/2} = 2.7$ to 6.7 d in sandy soil
(Dörfler et al. 1991); reported $t_{1/2} = 266 \text{ d in soil (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted,}$
Montgomery 1993);
reaction $t_{1/2} = 266 \text{ d (Mackay & Stiver 1991);}$
selected field $t_{1/2} = 400 \text{ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);}$
$t_{1/2} = 14 \text{ d for soil depth < 5 cm, } t_{1/2} = 90 \text{ d for 5–20 cm and } t_{1/2} = 180 \text{ d for >20 cm (Dowd et al. 1993) }$
$t_{1/2} = 14.5 \text{ and 16.0 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001) }$

Biota: $t_{1/2} = 22.1 \text{ h (mussels, Ernst 1977);}$
$t_{1/2} = 46 \text{ d (rainbow trout, Oliver & Niimi 1985);}$
biological half-lives for fishes: $t_{1/2} = 11 \text{ d for trout muscle, } t_{1/2} = 1 \text{ d for goldfish, } t_{1/2} < 1 \text{ d for sunfish and}$
t $t_{1/2} = 4 \text{ d for guppy (Niimi 1987);}$
$t_{1/2} = 678 \text{ h (azalea leaves, Bacci & Gaggi 1987);}$
biochemical $t_{1/2} = 266 \text{ d from screening model calculations (Jury et al. 1987b);}$
half-lives in plant surfaces at 20 ± 1°C: $t_{1/2} = 0.56 \text{ d in bean, } t_{1/2} = 0.40 \text{ d in turnips and } t_{1/2} = 0.31 \text{ d in oats}$
(Dörfler et al. 1991); elimination half-lives in the midge ($Chironomus riparius$) under varying sediment conditions: $t_{1/2} = 11 \text{ h for}$
water only system, $t_{1/2} = 10 \text{ h for screened system, } t_{1/2} = 9 \text{ h for 3% organic carbon system and } t_{1/2} = 6 \text{ h}$
for 15% organic carbon system (Lydy et al. 1992);
half-lives $t_{1/2}$ (in h) = 12.09 × L(% lipid) – 10.09, in different aquatic organisms (Geyer et al. 1997).
Average $t_{1/2} = 90 \text{ d (for pesticides used in conjunction with forest management, Neary et al. 1993).}$

### Table 18.1.1.54.1

Reported aqueous solubilities of lindane at various temperatures

<table>
<thead>
<tr>
<th>Richardson &amp; Miller 1960</th>
<th>Biggar &amp; Riggs 1974</th>
<th>OECD 1981</th>
</tr>
</thead>
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<tr>
<td>shake flask-UV spectro.</td>
<td>shake flask-GC</td>
<td>shake flask method</td>
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<tr>
<td>$t/°C$</td>
<td>$S/g \cdot m^{-3}$</td>
<td>$t/°C$</td>
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<tr>
<td>25</td>
<td>7.30</td>
<td>0.01µ</td>
</tr>
<tr>
<td>35</td>
<td>12.0</td>
<td>0.075</td>
</tr>
<tr>
<td>45</td>
<td>14.0</td>
<td>0.150</td>
</tr>
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</table>

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**FIGURE 18.1.1.54.1** Logarithm of mole fraction solubility \((\ln x)\) versus reciprocal temperature for lindane \((\gamma\text{-HCH})\).

<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>
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<tbody>
<tr>
<td>0</td>
<td>3.87 × 10⁻⁵</td>
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<td>1.701 × 10⁻⁶</td>
<td>20.03</td>
<td>0.00374</td>
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<tr>
<td>10</td>
<td>2.40 × 10⁻⁴</td>
<td>30</td>
<td>0.0171</td>
<td>-20</td>
<td>7.353 × 10⁻⁶</td>
<td>30.01</td>
<td>0.0225</td>
</tr>
<tr>
<td>20</td>
<td>1.253 × 10⁻³</td>
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<td>0.0608</td>
<td>-10</td>
<td>1.182 × 10⁻⁵</td>
<td>40.01</td>
<td>0.0281</td>
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<tr>
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<td>6.00 × 10⁻³</td>
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<td>0</td>
<td>4.489 × 10⁻⁴</td>
<td>30.01</td>
<td>0.0250</td>
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<td>40</td>
<td>0.0257</td>
<td>30 dry</td>
<td>0.0173</td>
<td>10</td>
<td>2.209 × 10⁻³</td>
<td>30.01</td>
<td>0.0281</td>
</tr>
<tr>
<td>50</td>
<td>0.1027</td>
<td>eq. 1 P/mmHg</td>
<td>0.0167</td>
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<td>9.395 × 10⁻³</td>
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<td>70</td>
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<td>eq. 1 P/mmHg</td>
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<td>80</td>
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<td></td>
<td>A</td>
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<td>90</td>
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<td>B</td>
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<td>60.00 × 10⁻³</td>
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<td>eq. 1 P/mmHg</td>
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<td>0.0167</td>
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**TABLE 18.1.1.54.2**

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

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

1. Balson 1947
   - efusion manometer
   - gas saturation-GC
   - temp range: 60–92°C
   - \(\Delta H_v = 101.13\) kJ/mol

2. Spencer & Cliath 1970
   - gas saturation-GC
   - temp range: 60–92°C
   - \(\Delta H_v = 115.06\) kJ/mol

3. Wania et al. 1994
   - gas saturation-GC
   - temp range: 20–200°C
   - \(\Delta H_v = 106.6\) kJ/mol

4. Boehncke et al. 1996
   - Knudsen effusion
   - temp range: 293–323 K
   - \(\Delta H_v = 97.7\) kJ/mol

**Lindane (\(\gamma\text{-HCH})\): solubility vs. \(1/T\)**

- Richardson & Miller 1960
- Biggar & Riggs 1974 (0.01 µ particle size)
- Biggar & Riggs 1974 (0.05 µ particle size)
- Biggar & Riggs 1974 (5.0 µ particle size)
- OECD 1981
- experimental data

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### TABLE 18.1.1.54.2 (Continued)

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<td>gas saturation-GC</td>
<td>Knudsen effusion</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
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<td>P/Pa</td>
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<td>125</td>
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2.

<table>
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<tr>
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<td>111</td>
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Combining the above 4 equations, the final equation:

\[
\text{log (P/kPa)} = 11.23 \pm 0.5 - \frac{(4832 \pm 150)}{(T/K)}
\]

for temperature range 310 to 384 K

\[
\Delta H_{\text{sub}} = 92.5 \text{ kJ/mol at 350 K}
\]

at 25°C P = 0.0104 Pa

(Continued)
### TABLE 18.1.1.54.2 (Continued)

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<tr>
<th>Giustini et al. 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B·(T/K) + C·(T/K)&lt;sup&gt;2&lt;/sup&gt; (5)</td>
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<table>
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<th><strong>A</strong></th>
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<th><strong>B</strong></th>
<th>4709</th>
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<tr>
<td><strong>A</strong></td>
<td>11.79</td>
<td><strong>B</strong></td>
<td>5025</td>
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</tbody>
</table>

for temp 323–370 K for temp 339–384 K

### FIGURE 18.1.1.54.2

Logarithm of vapor pressure versus reciprocal temperature for lindane (γ-HCH).

### TABLE 18.1.1.54.3

Reported Henry’s law constants of lindane (γ-HCH) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th><strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B·(T/K)</th>
<th><strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B·(T/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>log</strong> <strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B/(T/K)</td>
<td><strong>log</strong> <strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B/(T/K)</td>
</tr>
<tr>
<td><strong>ln</strong> (1/<strong>K</strong>&lt;sub&gt;n&lt;/sub&gt;) = A - B/(T/K)</td>
<td><strong>log</strong> (1/<strong>K</strong>&lt;sub&gt;n&lt;/sub&gt;) = A - B/(T/K)</td>
</tr>
<tr>
<td><strong>ln</strong> <strong>H</strong> = A - B/(T/K)</td>
<td><strong>log</strong> <strong>H</strong> = A - B/(T/K)</td>
</tr>
<tr>
<td><strong>K</strong>&lt;sub&gt;n&lt;/sub&gt; = A - B·(T/K) + C·(T/K)&lt;sup&gt;2&lt;/sup&gt; (5)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-GC</td>
<td>concentration ratio</td>
<td>air stripping-GC</td>
<td>air stripping/dynamic HS</td>
</tr>
<tr>
<td><strong>t</strong>/°C</td>
<td><strong>H</strong>/(Pa m&lt;sup&gt;3&lt;/sup&gt;/mol)</td>
<td><strong>t</strong>/°C</td>
<td><strong>H</strong>/(Pa m&lt;sup&gt;3&lt;/sup&gt;/mol)</td>
</tr>
<tr>
<td>distilled water</td>
<td>Green Bay</td>
<td>Lake Michigan</td>
<td>Lake Huron</td>
</tr>
<tr>
<td>0.5</td>
<td>0.0721</td>
<td>8.0</td>
<td>0.121</td>
</tr>
<tr>
<td>10</td>
<td>0.126</td>
<td>Lake Michigan</td>
<td>20</td>
</tr>
<tr>
<td>15</td>
<td>0.187</td>
<td>18.9</td>
<td>0.242</td>
</tr>
<tr>
<td>20</td>
<td>0.258</td>
<td>Lake Huron</td>
<td>35</td>
</tr>
<tr>
<td>23</td>
<td>0.339</td>
<td>18.5</td>
<td>0.236</td>
</tr>
</tbody>
</table>

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### TABLE 18.1.1.54.3 (Continued)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></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>25</td>
<td>0.353</td>
<td>22.3</td>
<td>0.310</td>
</tr>
<tr>
<td>35</td>
<td>0.624</td>
<td>22.3</td>
<td>0.301</td>
</tr>
<tr>
<td>45</td>
<td>1.170</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 4a</td>
<td>H/(Pa m³/mol)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>7.54 ± 0.54</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>2392 ± 160</td>
<td></td>
<td></td>
</tr>
<tr>
<td>seawater combined - both methods</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>0.0627</td>
<td></td>
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<tr>
<td>10</td>
<td>0.137</td>
<td></td>
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<tr>
<td>23</td>
<td>0.363</td>
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<td></td>
</tr>
<tr>
<td>35</td>
<td>0.996</td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>2.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td>eq. 4a</td>
<td>H/(Pa m³/mol)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>8.68 ± 0.96</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>2703 ± 276</td>
<td></td>
<td></td>
</tr>
<tr>
<td>for temp range 0.5–23°C</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 18.1.1.54.3** Logarithm of Henry’s law constant versus reciprocal temperature for lindane (γ-HCH).
TABLE 18.1.1.54.4
Reported octanol-water and octanol-air partition coefficients of lindane (γ-HCH) at various temperatures

<table>
<thead>
<tr>
<th>Temperature (t/°C)</th>
<th>log K&lt;sub&gt;OW&lt;/sub&gt;</th>
<th>log K&lt;sub&gt;OA&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paschke &amp; Schüürmann 1998 shake flask-GC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3.85</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>3.72</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>3.73</td>
<td></td>
</tr>
<tr>
<td>Shoeib &amp; Harner 2002 generator column-GC/MS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>8.6845</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>8.4493</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>8.2181</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>8.0643</td>
<td></td>
</tr>
</tbody>
</table>

Enthalpy of phase transfer:
\[ \Delta H_{OW}/(kJ \cdot mol^{-1}) = -10.40 \]

Entropy of phase transfer:
\[ \Delta S_{OW}/(J \cdot K^{-1} \cdot mol^{-1}) = 52.2 \]

\[
\log K_{OA} = A + B/(T/K)
\]

<table>
<thead>
<tr>
<th>Temperature (t/°C)</th>
<th>log K&lt;sub&gt;OA&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7.8473</td>
</tr>
<tr>
<td>25</td>
<td>7.849</td>
</tr>
</tbody>
</table>

Enthalpy of phase change
\[ \Delta H_{OA}/(kJ \cdot mol^{-1}) = 65.4 \]

FIGURE 18.1.1.54.4 Logarithm of K<sub>OW</sub> versus reciprocal temperature for lindane (γ-HCH).
FIGURE 18.1.54.5 Logarithm of $K_{OA}$ versus reciprocal temperature for lindane ($\gamma$-HCH).
18.1.1.55 Malathion

Common Name: Malathion
Chemical Name: S-[1,2-bis(ethoxycarbonyl)ethyl] O,O-dimethyl phosphorodithioate

Uses: as insecticide to control sucking and chewing insects and spider mites on vegetables, fruits, ornamentals, field crops in greenhouses, gardens and forestry; also used as acaricide.

CAS Registry No: 121-75-5
Molecular Formula: C_{10}H_{19}O_{6}PS_{2}
Molecular Weight: 330.358
Melting Point (°C):
1.4 (Lide 2003)
Boiling Point (°C):
120 (at 0.2 mmHg, Melnikov 1971; Freed et al. 1977)
156–157 (at 0.7 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
319.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
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):
145 (20°C, Macy 1948; Melnikov 1971; Spencer 1973)
145 (Spiller 1961; Willis & McDowell 1982)
150 (Hartley & Graham-Bryce 1980; Beste & Humbug 1983)
145 (22°C, Khan 1980)
143 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
145, 164 (20°C, 30°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
1.67 × 10⁻⁴ (20°C, Wolfdietrich 1965; Melnikov 1971; Montgomery 1993)
7.33 × 10⁻⁴ (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
2.90 × 10⁻³ (Woofford 1975)
1.30 × 10⁻³ (20°C, Hartley & Graham-Bryce 1980)
5.30 × 10⁻³ (30°C, Khan 1980)
9.20 × 10⁻⁴ (20°C, GC, Seiber et al. 1981)
1.05 × 10⁻³ (gas saturation-GC, Kim et al. 1984; Kim 1985)
0.60 × 10⁻³ (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984, Kim 1985)
Insecticides

0.67 × 10⁻³ (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
5.30 × 10⁻³ (30°C, Hartley & Kidd 1987; Tomlin 1994)
4.70 × 10⁻³ (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
0.0063 (liquid P L, GC-RT correlation; Donovan 1996)
1.07 × 10⁻³ (selected, Halfon et al. 1996)
0.00174 (gradient GC method; Tsuzuki 2000)
1.78 × 10⁻³; 1.35 × 10⁻³, 2.51 × 10⁻³ (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.038 (calculated-P/C, Mackay & Shiu 1981)
2.30 × 10⁻³ (20°C, calculated-P/C, Suntio et al. 1988)
3.22 × 10⁻³ (calculated-P/C, Taylor & Glotfelty 1988)
2.03 × 10⁻³ (calculated-P/C, Howard 1991)
4.96 × 10⁻⁴ (calculated-bond contribution method, Meylan & Howard 1991)
4.9 × 10⁻⁴ (23°C, quoted, Schomburg et al. 1991)
4.9 × 10⁻⁴ (Montgomery 1993)

Octanol/Water Partition Coefficient, log K OW:
2.89 (20°C, shake flask-GC, Chiou et al. 1977)
2.89 (shake flask-GC, Freed et al. 1979; Yoshioka et al. 1986)
2.36 (Hansch & Leo 1979, 1985)
2.36 (Rao & Davidson 1980)
2.82 (shake flask-GC/FID, Hermens & Leeuwangh 1982)
2.94 (shake flask/slow-stirring method-GC, De Bruijn et al. 1991)
2.75 (Worthing & Hance 1991; Tomlin 1994)
2.36–2.89 (Montgomery 1993)
2.68 (RP-HPLC-RT correlation, Saito et al. 1993)
2.18 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.36 (recommended, Sangster 1993)
2.36 (selected, Hansch et al. 1995)
2.18 (RP-HPLC-RT correlation, Finizio et al. 1997)
3.57 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
1.11 (carp, calculated from k 1 of Bender 1969, McLeese et al. 1976)
–4.74 (beef biotransfer factor logB b, correlated-K OW, Pasarela et al. 1962)
0.867, 1.47 (lake trout, coho salmon, Howard 1991)
2.94, 2.98 (white shrimp, brown shrimp, Conte & Parker 1975)
1.57 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
0.40 ( Triaenodes tardus, Belluck & Felsot 1981)
1.54 (willow shiner, Tsuda et al. 1989)
0.85 (carp, wet wt. basis, De Bruijn & Hermens 1991)
2.00 (topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
1.57 (Pait et al. 1992)

Sorption Partition Coefficient, log K OC:
2.45 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
3.26 (av. soils/sediments, Rao & Davidson 1980)
3.25 (Rao & Davidson 1980)
3.25 (Karickhoff 1981)
2.83, 3.29, 2.50 (estimated-S, calculated-S and mp, estimated-K OW, Karickhoff 1981)
2.36 (Bomberger et al. 1983)
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

**Volatilization:** $t_{1/2} = 131$ d, based on volatilization rate from water with a wind speed of 0–2.5 m/s (Sanders & Seiber 1984; quoted, Howard 1991).

**Photolysis:** $t_{1/2} = 15$ h for direct sunlight photolysis in aqueous media (Wolfe et al. 1976)
$t_{1/2} = 900$ h in distilled water at pH 6 with wavelength $\lambda > 290$ nm; $t_{1/2} = 16$ h by sunlight in a natural water from Suwannee River (Wolfe et al. 1977)
$t_{1/2} = 990–20000$ h for both atmospheric and aqueous photolysis, based on experimental photolysis rate constant in aqueous solution at pH 6 exposure to $>290$ nm under summer sunlight at 40°N (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 $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:
photooxidation $t_{1/2} = 1.0–9.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)
$k_{OH}(calc) = 64 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Winer & Atkinson 1990) calculated lifetime $\tau = 3$ h for reaction with OH radical in the troposphere (Atkinson et al. 1992)

**Hydrolysis:** $t_{1/2} = 10.5$ d at pH 7.4 and 20°C (Freed et al. 1977, 1979; Montgomery 1993)
$t_{1/2} = 120$ d at pH 6.1 and $t_{1/2} = 11$ d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation method for hydrolysis rates determination (Freed et al. 1979)

**Biodegradation:** $k = 6.2 \times 10^{-8}$ mL cell$^{-1}$ d$^{-1}$ (Paris et al. 1975; quoted, Scow 1982)
$k = 5.0 \times 10^{-8}$ mL cell$^{-1}$ d$^{-1}$ (Baughman & Lassiter 1978; quoted, Scow 1982)
$k = 2.6 – 16.1 \times 10^{-7}$ mL cell$^{-1}$ d$^{-1}$ (Paris et al. 1978; quoted, Scow 1982);
$k = 1.4$ d$^{-1}$ in soil (Rao & Davidson 1980; quoted, Scow 1982)

**Biotransformation:** transformation rate $k = 7.8 \times 10^{-3}$ mg (mg fungi)$^{-1}$ h$^{-1}$ by a fungi *Aspergillus oryzae* at 28°C in aqueous solution (Lewis et al. 1975)
$k = 1.9 \times 10^{-1}$ mg (mg fungi)$^{-1}$ d$^{-1}$ in aquatic systems (Lewis et al. 1975; quoted, Scow 1982)

**Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:**
$k_1 = 1.07$ d$^{-1}$ (carp, Bender 1969; quoted, McLeese et al. 1976)
$k_2 = 0.08$ d$^{-1}$ (carp, calculated. from $k_1$ of Bender 1969, McLeese et al. 1976)
$k_2 = 0.49$ h$^{-1}$ (willow shiner, Tsuda et al. 1989)
Insecticides

Half-Lives in the Environment:

Air: $t_{1/2} = 1.0–9.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991); calculated lifetime of 3 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992).

Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);
$\bar{t}_{1/2} = 100–1236$ h, based on unacclimated aerobic river die-away test data and estuarine water grab sample data (Howard et al. 1991);
$\bar{t}_{1/2} = 1.65$ d in Indian River water, at 24 ppt salinity and pH 8.16 (Wang & Hoffman 1991);
$\bar{t}_{1/2} = 212$ d at 6°C, $\bar{t}_{1/2} = 42$ d at 22°C in darkness for Milli-Q water, pH 6.1; $\bar{t}_{1/2} = 55$ d at 6°C, $\bar{t}_{1/2} = 19$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $\bar{t}_{1/2} = 53$ d at 6°C, $\bar{t}_{1/2} = 7$ d at 22°C in darkness for filtered river water at pH 7.3; $\bar{t}_{1/2} = 41$ d at 6°C, $\bar{t}_{1/2} = 6$ d at 22°C in darkness, $\bar{t}_{1/2} = 14$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995)

Biodegradation $\bar{t}_{1/2}($aerobic$) = 4.2$ d, $\bar{t}_{1/2}($anaerobic$) = 17$ d, hydrolysis $\bar{t}_{1/2} = 3200$ d at pH 7 and $\bar{t}_{1/2} = 0.0006$ d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $\bar{t}_{1/2} = 200–2472$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $\bar{t}_{1/2} = 2$ d in sediment suspension (Cotham & Bidleman 1989)
first-order degradation $k = 0.902$ d$^{-1}$ with $\bar{t}_{1/2} = 0.8$ d under aerobic conditions, $k = 0.302$ d$^{-1}$ with $\bar{t}_{1/2} = 2.3$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.506$ d$^{-1}$ with $\bar{t}_{1/2} = 1.4$ d under aerobic conditions, $k = 0.431$ d$^{-1}$ with $\bar{t}_{1/2} = 1.6$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: estimated persistence of one week (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);
$\bar{t}_{1/2} = 72–168$ h, based on unacclimated aerobic soil grab sample data (Walker & Stojanovic 1973; quoted, Howard et al. 1991); biodegradation rate constant of 1.4 d$^{-1}$ in soil (Rao & Davidson 1980; quoted, Scow 1982); non-persistent in soil with $\bar{t}_{1/2} < 20$ d (Willis & McDowell 1982); $\bar{t}_{1/2} = 1$ in screening model simulations (Jury et al. 1987b); Degradation $\bar{t}_{1/2} = 8$ d in a coarse sandy soil, $\bar{t}_{1/2} = 19$ d in sandy loam (Kjeldsen et al. 1990) selected field $\bar{t}_{1/2} = 1.0$ d (Wauchope et al. 1992; Dowd et al. 1993; Halfon et al. 1996; Hornsby et al. 1996); soil $\bar{t}_{1/2} = 11$ d (Puit et al. 1992); $\bar{t}_{1/2} = 1$ d for soil depth $< 5$ cm, $\bar{t}_{1/2} = 7$ d for soil depth $5–20$ cm and $\bar{t}_{1/2} = 14$ d for soil depth $>20$ cm (Dowd et al. 1993).

Biota: biochemical $\bar{t}_{1/2} = 1$ d from screening model calculations (Jury et al. 1987b); excretion $\bar{t}_{1/2} = 1.4$ h (willow shiner, Tsuda et al. 1989); average $\bar{t}_{1/2} = 20$ d in the forest (USDA 1989; quoted, Neary et al. 1993).
18.1.1.56 Methiocarb

Common Name: Methiocarb

Synonym: Bayer 37344, Draza, EnsuroL, Mercaptodimethur, Mesurol, Mesurol Phenol, metmercapturon

Chemical Name: 4-methylthio-3,5-xylyl methylcarbamate; 3,5-dimethyl-4-(methylthio)phenol methylcarbamate

Uses: Insecticide/Acaricide/Molluscicide/Repellent; to control slugs and snails in a wide range of agricultural situations; broad range control of lepidoptera, coleoptera, diptera, and homoptera and spider mites in pome fruit, stone fruit, citrus fruit, strawberries, hops, potatoes, beet, maize, oilseed rape, vegetables and ornamentals; also used as a bird repellent.

CAS Registry No: 2032-65-7

Molecular Formula: C_{11}H_{15}NO_{2}S

Molecular Weight: 225.308

Melting Point (°C):
- 120 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):
- 1.236 (Tomlin 1994)

Molar Volume (cm³/mol):
- 261.4 (calculated-Le Bas method at normal boiling point)
- 182.3 (calculated-density)

Dissociation Constant, pKₐ:

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: 0.117 (mp at 120°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 27 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
- 0.015 (60°C, Hartley & Kidd 1987)
- 1.5 × 10⁻⁵ (20°C, Tomlin 1994)
- 3.6 × 10⁻⁵ (Tomlin 1994)
- 0.016 (20–25°C, selected, Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol):
- 0.120 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
- 2.92 (shake flask as per Fujita et al. 1964; Briggs 1981)
- 2.92 (selected, Magee 1991)
- 3.34 (Tomlin 1994)
- 2.92 (recommended, Hansch et al. 1995)
- 2.82 (Pomona-database, Müller & Kördel 1996)
- 2.95 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
Bioconcentration Factor, log BCF:

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

- 2.32 (20°C, sorption isotherm, converted from log $K_{OM}$ of 2.08, Briggs 1981)
- 2.08, 2.33 (reported as log $K_{OM}$, converted from $K_{OM}$ multiplied by 1.724, Magee 1991)
- 2.82 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
- 2.32 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 2.82, 2.26 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.48 (20–25°C, estimated, Hornsby et al. 1996)
- 3.12, 2.45, 2.38, 2.88, 2.80 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 2.25 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
- 2.32; 2.23, 2.22 (soil, quoted exptr.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

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

Photolysis: photodegradation half-life of 6–16 d (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_\frac{1}{2} = 30$ d (20–25°C, estimated, Hornsby et al. 1996).
18.1.1.57 Methomyl

Common Name: Methomyl
Synonym: Du Pont 1179, ENT 27341, Lannate, Mesomile, Nu-bait II, Nudrin, SD 14999, WL 18236
Chemical Name: S-methyl-N-(methylcarbamoyloxy) thioacetimidate; methyl-N-(((methylamino)-carbonyl)oxy) ethan-imidothioate
Uses: insecticide/acaricide; control a wide range of insects and spider mites in fruit, vines, olives, hops, vegetables, ornamentals, field crops, cucurbits, flax, cotton, soya beans, etc.; also used for control of flies in animal and poultry houses and dairies.
CAS Registry No: 16752-77-5
Molecular Formula: C₅H₁₀N₂O₂S
Molecular Weight: 162.210
Melting Point (°C):
78 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
179.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔHₕus (kJ/mol):
22.267 (DSC method, Plato 1972)
Entropy of Fusion, ΔSₕus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕus = 56 J/mol K), F: 0.302 (mp at 78°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
10000 (Kenaga 1980a; Kenaga & Goring 1980)
> 1000 (20°C, shake flask-GC, Bowman & Sans 1983a)
57900 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
58000 (20–25°C, selected, Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
3.47 × 10⁻³ (20°C, Hartley & Graham-Bryce 1980)
6.66 × 10⁻³ (Khan 1980; Spencer 1982)
0.162 (30°C, GC, Seiber et al. 1981)
6.67 × 10⁻³ (Worthing 1983)
3.47 × 10⁻³ (20°C, selected exptl. value, Kim 1985)
7.53 × 10⁻², 1.99 × 10⁻² (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
6.67 × 10⁻³ (20–25°C, selected, Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.82 × 10⁻⁵ (calculated, Lyman et al. 1982)
6.50 × 10⁻⁵ (20°C, calculated-P/C, Suntio et al. 1988)
6.48 × 10⁻⁵ (calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.30 (Dow Chemical data, Kenaga & Goring 1980)
- 1.08 (Rao & Davidson 1980)
- 0.131 (22°C, shake flask-GC, Bowman & Sans 1983b)
- 0.60 (shake flask-HPLC, Drabel & Bachmann 1983)
- 0.60 (Hansch & Leo 1985)
- 0.13, 1.08 (Montgomery 1993)
- 0.60 (recommended, Sangster 1993)
- 0.09 (Tomlin 1994)
- 0.60 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 0.477, 0.903 (calculated-S, calculated-$K_{OC}$, Kenaga 1980)
- 0.230, 0.110 (calculated-$K_{OW}$, calculated-S, Howard 1991)

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

- 2.20 (soil, Fung & Uren 1977)
- 1.45 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 1.71; 1.00 (calculated-$K_{OC}$, calculated-S, Lyman et al. 1982)
- 2.20 (Worthing 1983)
- 1.08 (soil, calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
- 1.86, 2.20 (Montgomery 1993)
- 1.86 (estimated-chemical structure, Lohninger 1994)
- 1.86 (Tomlin 1994)
- 1.30 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.86 (soil, 20–25°C, selected, Hornsby et al. 1996)
- 1.16, 1.62 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

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

Volatileization:

Photolysis:

Oxidation: photooxidation $t_{1/2} \sim 1.14$ months, based on vapor-phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Hydrolysis: experimental $t_{1/2} = 262$ d from rate constant $k = 8.9 \times 10^{-5}$ h$^{-1}$ has been determined in pure water at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard 1991; Montgomery 1993).

Biodegradation: rate constants $k = -0.000215$ h$^{-1}$ in nonsterile sediment, $k = -0.000747$ h$^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000175$ h$^{-1}$ in nonsterile water and $k = -0.000383$ h$^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} \sim 1.14$ months, based on rate constant $k = 2.919 \times 10^{-13}$ cm$^3$/molecules for the vapor-phase reaction with $8 \times 10^7$/cm$^3$ hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Surface water: experimental $t_{1/2} = 262$ d has been determined in pure water at 25°C (Ellington et al. 1988; quoted, Howard 1991).

Ground water: $t_{1/2} < 0.2$ d in ground water samples (Smelt et al. 1983; quoted, Tomlin 1994).

Sediment:

Soil: field $t_{1/2} = 30$ d (20–25°C, selected, Hornsby et al. 1996).

Biota: $t_{1/2} \sim 3–5$ d in plants following leaf application (Harvey & Reiser 1973; quoted, Tomlin 1994);

- $t_{1/2} = 0.4–8.5$ d on cotton plants, $t_{1/2} = 0.8–1.2$ d on mint plants and $t_{1/2} \sim 2.5$ d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).
18.1.1.58 Methoxychlor

Common Name: Methoxychlor
Synonym: Chemform, Dimethoxy-DDT, DMDT, DMTD, ENT 1716, Maralate, Marlate, Methorcide, Methoxo, Metox, Moxie NCI-C00497
Chemical Name: 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)ethane; 1,1′-(2,2,2-trichloroethylidene)bis[4-methoxybenzene]
Uses: insecticide to control mosquito larvae, house flies, and other insect pests in field crops, fruits, and vegetables; also to control ectoparasites on cattle, sheep, and goats.
CAS Registry No: 72-43-5
Molecular Formula: C16H15Cl3O2
Molecular Weight: 345.648
Melting Point (°C): 87 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

   354.3 (calculated-Le Bas method at normal boiling point)
   245.1 (calculated-density)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

   27.614 (DSC method, Plato & Glasgow 1969)
   23.88 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°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):

   0.10* (shake flask-UV, measured range 25–45°C, Richardson & Miller 1960)
   0.62 (Karpoo et al. 1970)
   0.003, 0.01, 0.045* (particle size of 0.01, 0.05 and 5.0μ; shake flask-GC, measured range 15–45°C, Biggar & Riggs 1974)
   0.10 (generator column-GC/ECD, Weil et al. 1974)
   0.12 (shake flask-GC/ECD, Zepp et al. 1976, Karickhoff et al. 1979; Karickhoff 1981)
   0.1–0.25 (Wauchope 1978)
   0.10 (Weber et al. 1980)
   0.10 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
   0.04 (24°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
< 1.33 × 10⁻⁴ (20–25° C, Weber et al. 1980)
1.910 × 10⁻⁴ (estimated, Howard 1991)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

   1.60 (estimated, Hine & Mookerjee 1975; quoted, Howard 1991)
   0.999 (calculated-P/C, this work)
   0.0206 (wetted wall column-GC, Altschuh et al. 1999)
### Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.68</td>
<td>(HPLC-RT correlation, Veith &amp; Morris 1978)</td>
</tr>
<tr>
<td>5.08</td>
<td>(shake flask-UV, Karickhoff et al. 1979; Karickhoff 1981)</td>
</tr>
<tr>
<td>4.30</td>
<td>(HPLC-RT correlation, Veith et al. 1979, 1980)</td>
</tr>
<tr>
<td>4.20</td>
<td>(Mackay et al. 1980)</td>
</tr>
<tr>
<td>4.83</td>
<td>(Belluck &amp; Felsot 1981)</td>
</tr>
<tr>
<td>4.51</td>
<td>(HPLC-$k'$ correlation, McDuffie 1981)</td>
</tr>
<tr>
<td>4.83</td>
<td>(shake flask-UV, Nishimura &amp; Fujita 1983)</td>
</tr>
<tr>
<td>4.68–5.08</td>
<td>(Hansch &amp; Leo 1985)</td>
</tr>
<tr>
<td>4.91, 4.26</td>
<td>(shake flask, RP-TLC-RT correlation, Renberg et al. 1985)</td>
</tr>
<tr>
<td>3.31, 5.08</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>4.95</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>5.08</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>4.58</td>
<td>(RP-HPLC-RT correlation, Finizio et al. 1997)</td>
</tr>
</tbody>
</table>

### Octanol/Air Partition Coefficient, $\log K_{\text{oa}}$:

### Bioconcentration Factor, $\log BCF$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>–1.70</td>
<td>(bioaccumulation factor logBF, adipose tissue in female Albino rats, Harris et al. 1974)</td>
</tr>
<tr>
<td>4.68, 3.08, 3.72, 3.92</td>
<td>($\text{Bacillus subtilis}$, $\text{Flavobacterium harrisonii}$, $\text{Aspergillus sp.}$, $\text{Chlorella pyrenoidosa}$, Paris et al. 1975; Paris &amp; Lewis 1976)</td>
</tr>
<tr>
<td>4.40</td>
<td>(bacterial sorption, Paris &amp; Lewis 1976)</td>
</tr>
<tr>
<td>2.14</td>
<td>(sheephead minnow, Farrish et al. 1977)</td>
</tr>
<tr>
<td>3.92, 3.72</td>
<td>(algae, fungi, Wolfe et al. 1977)</td>
</tr>
<tr>
<td>3.92</td>
<td>(fathead minnows, 32 d exposure, Veith et al. 1979, 1980)</td>
</tr>
<tr>
<td>3.70–3.93, 2.54–3.05</td>
<td>(snail, Stonefly, Anderson &amp; Defoe 1980)</td>
</tr>
<tr>
<td>2.27, 3.19</td>
<td>(fish: flowing water, static water; Kenaga 1980b; Kenaga &amp; Goring 1980)</td>
</tr>
<tr>
<td>4.21, 3.91</td>
<td>(calculated-S, $K_{\text{OC}}$, Kenaga 1980)</td>
</tr>
<tr>
<td>1.15</td>
<td>($\text{Triaendoes tardus}$, Belluck &amp; Felsot 1981)</td>
</tr>
<tr>
<td>4.20, 3.04, 3.91</td>
<td>(estimated-S, $K_{\text{OW}}$, $K_{\text{OC}}$, Bysshe 1982)</td>
</tr>
<tr>
<td>3.92</td>
<td>(fathead minnows, Veith &amp; Kosian 1983)</td>
</tr>
<tr>
<td>4.08</td>
<td>(mussel, Renberg et al. 1985)</td>
</tr>
<tr>
<td>3.18</td>
<td>(soft clams, Hawker &amp; Connell 1986)</td>
</tr>
<tr>
<td>3.92</td>
<td>(calculated, Isnard &amp; Lambert 1988)</td>
</tr>
<tr>
<td>5.40</td>
<td>(calculated field bioaccumulation, Thomann 1989)</td>
</tr>
<tr>
<td>5.29</td>
<td>(rainbow trout lipid base, estimated, Noegrohati &amp; Hammers 1992)</td>
</tr>
<tr>
<td>3.98; 4.05</td>
<td>($\text{Oncorhynchus mykiss}$, wet wt. basis: quoted exp.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)</td>
</tr>
</tbody>
</table>

### Sorption Partition Coefficient, $\log K_{\text{oc}}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.79</td>
<td>(water-sediment, Wolfe et al. 1977)</td>
</tr>
<tr>
<td>4.90</td>
<td>(av. for isotherms on sediments, Karickhoff et al. 1979)</td>
</tr>
<tr>
<td>3.99–4.61, 4.90–5.00, 4.86–4.96</td>
<td>(sand, fine silt, clay Karickhoff et al. 1979)</td>
</tr>
<tr>
<td>4.90</td>
<td>(soil, quoted, Kenaga 1980a, b; Kenaga &amp; Goring 1980; Bysshe 1982)</td>
</tr>
<tr>
<td>5.03</td>
<td>(soil, calculated-S as per Kenaga &amp; Goring 1978, Kenaga 1980)</td>
</tr>
<tr>
<td>6.04</td>
<td>(calculated-S, Mill et al. 1980)</td>
</tr>
<tr>
<td>4.90</td>
<td>(av. soils/sediments, Rao &amp; Davidson 1980)</td>
</tr>
<tr>
<td>4.67, 4.69, 5.54</td>
<td>(estimated-S, $K_{\text{OW}}$, $S$ and mp, Karickhoff 1981)</td>
</tr>
<tr>
<td>4.26</td>
<td>(soil, screening model calculations, Jury et al. 1987b)</td>
</tr>
<tr>
<td>4.99</td>
<td>(RP-HPLC-$k'$ correlation, cyanopropyl column, Hodson &amp; Williams 1988)</td>
</tr>
<tr>
<td>4.63</td>
<td>(soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)</td>
</tr>
<tr>
<td>4.90</td>
<td>(estimated-QSAR and SPARC, Kollig 1993)</td>
</tr>
<tr>
<td>4.90, 4.95</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>4.90</td>
<td>(soil, calculated-MCI $'\chi'$, Sabljic et al. 1995)</td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Volatilization: \( t_{1/2} = 4.5 \) d from water was estimated based on Henry’s law constant for a model river 1 m deep with a current of 1 m/s and a wind speed of 3 m/s (Howard 1991).

Photolysis: midsummer direct photolysis \( t_{1/2} = 690 \) h in water, \( t_{1/2} = 4100 \) h in hydrocarbon media; midday \( t_{1/2} = 1100 \) h average over all seasons in water at latitude 40°N, daily average direct photolysis \( t_{1/2} = 4.5 \) months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

photodecomposition \( t_{1/2} > 300 \) h in distilled water, \( t_{1/2} = 2.2 \) h in Suwannee River water, \( t_{1/2} = 5.4 \) h in Tombigbee River water, \( t_{1/2} = 2.9 \) h in Alabama River water with methoxychlor at 40 ppb under sunlight (Zepp et al. 1976)

\( t_{1/2} = 300–2070 \) h in both air and natural water, based on measured photolysis rates in distilled water under midday sunlight and adjusted for approximate winter sunlight intensity (Howard et al. 1991).

Oxidation:

photooxidation \( t_{1/2} = 2.2–5.4 \) h in natural water, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

photooxidation \( t_{1/2} \sim 1.12–11.2 \) h in air, based on rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

\( k(aq.) = (270 \pm 80) \text{ M}^{-1} \text{s}^{-1} \) for direct reaction with ozone in water at pH 2 and 24 ± 1°C, with \( t_{1/2} = 21 \) min at pH 7 (Yao & Haag 1991).

\( k_{OH(aq.)} = 2 \times 10^{10} \text{ M}^{-1} \text{s}^{-1} \) for the reaction with hydroxyl radicals in aqueous solutions at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: \( k(alkaline) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{s}^{-1} \) with \( t_{1/2} = 2100 \) d at 27°C, \( k(neutral) = 2.2 \times 10^{-8} \text{ s}^{-1} \) at pH 3–7 corresponds to a \( t_{1/2} = 367 \) d at pH 9 and 27°C (Wolf et al. 1977)

Overall rate constant \( k = 5.5 \times 10^{-8} \text{ s}^{-1} \) with \( t_{1/2} = 147 \) d; \( k = 3.0 \times 10^{-8} \text{ s}^{-1} \) with \( t_{1/2} = 270 \) d at 25°C and pH 7 (Mabey & Mill 1978)

\( k(alkaline) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{s}^{-1} \), \( k(neutral) = 2.2 \times 10^{-8} \text{ s}^{-1} \), \( 1 \times 10^{-8} \text{ M} \) in water at 27°C (Harris 1982)

\( t_{1/2} = 1.05 \) yr, based on neutral and base catalyzed hydrolysis rate constants Howard et al. 1991

\( k = 0.60 \text{ yr}^{-1} \) at pH 7 and 25°C (Kollig 1993)

\( t_{1/2} = 370 \) d at pH 2, \( t_{1/2} = 370 \) d at pH 7 and \( t_{1/2} = 270 \) d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: \( t_{1/2}(aq. \text{ aerobic}) = 4320–8760 \) h (6 months to 1 yr), based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

\( t_{1/2}(aq. \text{ anaerobic}) = 1200–4320 \) h (50 d to 6 months), based on anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

\( k = -0.00236 \text{ h}^{-1} \) in nonsterile sediment and \( k = -0.000639 \text{ h}^{-1} \) in sterile sediment by shake-tests at Range Point and \( k = -0.000139 \text{ h}^{-1} \) in nonsterile water and \( k = -0.0000327 \text{ h}^{-1} \) in sterile water by shake-tests at Range Point (Walker et al. 1988)

\( t_{1/2}(aerobic) = 180 \) d, \( t_{1/2}(anaerobic) = 50 \) d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

\( k_1 = 14.4–37.5 \text{ h}^{-1} \) (Chironomus tentans larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

\( k_1 = 11.4–82.0 \text{ h}^{-1} \) (Chironomus tentans larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

\( k_1 = 35.8–54.9 \text{ h}^{-1} \) (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

\( k_1 = 35.8–54.9 \text{ h}^{-1} \) (Chironomus tentans larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

\( k_2 = 45.4–38.6 \text{ h}^{-1} \) (Chironomus tentans larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

\( k_2 = 0.030 \text{ h}^{-1} \) (Chironomus tentans larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: \( t_{1/2} \sim 1.12–11.2 \) h, based on rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
Surface water: midsummer direct photolysis $t_\text{d} = 690$ h in water; midday $t_\text{d} = 1100$ h average over all seasons in water at latitude 40°N, daily average direct photolysis $t_\text{d} = 4.5$ months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

$\tau_\text{d} = 2.2$–5.4 h, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

measured $k = (270 \pm 80)$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and 24 ± 1°C, with a $\tau_\text{d} = 2.1$ min at pH 7 (Yao & Haag 1991)

biodegradation $\tau_\text{d(aerobic)} = 180$ d, $\tau_\text{d(anaerobic)} = 50$ d, hydrolysis $\tau_\text{d} = 370$ d at pH 2, $\tau_\text{d} = 370$ d at pH 7 and $\tau_\text{d} = 270$ d at pH 12 in natural waters (Capel & Larson 1995).

Ground water: $\tau_\text{d} = 1200$–8760 h, based on aerobic and anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991).

Sediment:
Soil: $\tau_\text{s} = 1.5$ wk at pH 4.7 and 6.5 and $\tau_\text{s} = 1.0$ wk at pH 7.8 (Carlo et al. 1952; quoted, Kaufman 1976);

$\tau_\text{s} = 4320$–8760 h, based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991);

$\tau_\text{s} = 42$ d in screening model calculations (Jury et al. 1987b);

selected field $\tau_\text{s} = 120$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $\tau_\text{b} = 9.6$ h in pond sediment-water, $\tau_\text{b} = 23.2$ h in sand-water system (Chironomus tentans larvae, Muir et al. 1983);

$\tau_\text{b} = 0.4$–8.5 d on cotton plants, $\tau_\text{b} = 0.8$–1.2 d on mint plants and $\tau_\text{b} \sim 2.5$ d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).

### TABLE 18.1.158.1

Reported aqueous solubilities of methoxychlor at various temperatures

<table>
<thead>
<tr>
<th>Richardson &amp; Miller 1960</th>
<th>Biggar &amp; Riggs 1974</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-UV spec.</td>
<td>shake flask-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g·m}^{-3}$</td>
</tr>
<tr>
<td></td>
<td>particle size</td>
</tr>
<tr>
<td>25</td>
<td>0.10</td>
</tr>
<tr>
<td>35</td>
<td>0.20</td>
</tr>
<tr>
<td>45</td>
<td>0.40</td>
</tr>
<tr>
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</tr>
</tbody>
</table>
FIGURE 18.1.1.58.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for methoxychlor.
18.1.1.59 Mevinphos

Common Name: Mevinphos
Synonym: Apavinfos, CMDP, Compound 2046, Duraphos, ENT 22374, Fosdrin, Gesfid, Gestid, Meniphos, Menite, NA 2783, OS 2046, PD 5, Phosdrin, Phosfene

Chemical Name: 2-carbomethoxy-1-methylvinyl dimethyl phosphate; 1-methoxycarbonyl-1-propen-2-yl dimethyl phosphate; methyl-3-(dimethoxyphosphinoyloxy)but-2-enoyl ester 2-carbomethoxy-1-methylvinyl dimethyl phosphate

Uses: contact insecticide and acaricide to control chewing insects and spider mites in fruits, vegetables, and ornamentals.

CAS Registry No: 7786-34-7 [formerly 298-01-1 for (E) isomer & 338-45-4 for (Z) isomer] for cis-isomer and 338-45-4 for trans-isomer

Molecular Formula: C$_7$H$_{13}$O$_6$P
Molecular Weight: 224.1 48

Melting Point (°C):
-56.1 (Montgomery 1993; Lide 2003)
21 ((E) isomer, Lide 2003)
6.9 ((Z) isomer, Lide 2003)

Boiling Point (°C)
99–103 (at 0.03 mmHg, Martin 1971; Freed et al. 1977; Milne 1995)
76.0 (at 0.2 mmHg, Melnikov 1971; Freed et al. 1979)
110 (at 1.6 mmHg, Hartley & Kidd 1987)
106–107.5 (at 1 mmHg, Montgomery 1993)

Density (g/cm$^3$ at 20°C):
1.24 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.25 (Montgomery 1993)
1.235, 1.245 ((E) isomer, (Z) isomer, Tomlin 1995)

Molar Volume (cm$^3$/mol):
180.7 (calculated from density)

Dissociation Constant, pK$_a$:

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/m$^3$ or mg/L at 25°C or as indicated):
miscible (Spencer 1973; Worthing 1979; Freed et al. 1979)
> 2000 (shake flask-GC, Bowman & Sans 1983a)
miscible (Hartley & Kidd 1987; Tomlin 1994)
miscible (Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C or as indicated):
0.293 (20°C, Eichler 1965)
0.293 (20–25°C, Melnikov 1971)
0.757 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
0.017 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.0173 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.293 (20°C, Montgomery 1993)

Henry’s Law Constant (Pa·m$^3$/mol):
6.35 × 10$^{-6}$ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 0.845 (Melnikov 1971)
- 0.954 (Freed et al. 1977)
- 0.550 (selected, Dao et al. 1983)
- 1.20 (shake flask, Log P Database. Hansch & Leo 1987)
- 0.200 (selected, Boehncke et al. 1990)
- 0.130 (Tomlin 1994)
- 1.20 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

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

- 1.64 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.64 (estimated-chemical structure, Lohninger 1994)
- 2.30 (soil, calculated-MCI $\chi_1$, Sabljic et al. 1995)
- 2.12, 1.56 (soil, cis-mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.28, 1.67 (soil, trans-mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

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

Hydrolysis: $t_{1/2} = 1.8$ h for cis- and $t_{1/2} = 3.0$ h for trans-isomer at pH 11.6 (Casida et al. 1956; quoted, Montgomery 1993);

- $t_{1/2} = 30–35$ d (Melnikov 1971; quoted, Freed et al. 1977);
- $t_{1/2} = 120$ d at pH 6, $t_{1/2} = 35$ d at pH 7, $t_{1/2} = 3$ d at pH 9, and $t_{1/2} = 1.4$ h at pH 11 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Air:
Ground water:
Sediment:
Soil: selected field $t_{1/2} = 3$ d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota: estimated $t_{1/2} = 19 \pm 2$ and $24 \pm 7$ h in lettuce in the summer and $t_{1/2} = 20 \pm 11$ h in the fall, $t_{1/2} = 50$ h in cauliflower in the summer and $t_{1/2} = 18 \pm 1$ h in the fall, $t_{1/2} = 25 \pm 2$ h in celery in the summer and $t_{1/2} = 16$ h in the fall (Spencer et al. 1992)
Insecticides

18.1.1.60 Mirex

Common Name: Mirex
Synonym: Bichlorendo, Declarane, ENT 25719, Ferriamicide, Paramex, Perclordecone
Chemical Name: 1,1a,2,3,3a,4,5,5a,5b,6-dodecachloro-octahydro-1,3,4-methano-1H-cyclobuta(cd) pentalene; dodecachloro-pentacyclodecane
Uses: Insecticide.
CAS Registry No: 2385-85-5
Molecular Formula: C_{10}Cl_{12}
Molecular Weight: 545.542
Melting Point (°C):
Boiling Point (°C):
403.2 (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: 3.1 × 10⁻⁵ (mp at 485°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.001 (from D. Dollar of Miss. State Chem. Lab. unpublished results, Alley 1973)
0.085 (shake flask-LSC, Metcalf et al. 1973)
0.60 (Neely 1978; quoted, Kenaga 1980; Kenaga & Goring 1980)
7.0 × 10⁻⁵ (22°C, shake flask-GC, Smith et al. 1978)
0.02 (24°C, Verschueren 1983)
7.0 × 10⁻⁵ (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):
8.0 × 10⁻⁴ (50°C, Smith, et al. 1978)
1.3 × 10⁻⁴ (20°C, Smith et al. 1978)
1.0 × 10⁻⁴ (20°C, selected, Suntio et al. 1988)
9.0 × 10⁻⁷ (10°C, estimated, McLachlan et al. 1990)
2.5 × 10⁻³, 2.9 × 10⁻⁴, 2.8 × 10⁻⁴ (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
5.2 × 10⁻⁵ (12°C, extrapolated supercooled liquid value, Hinckley et al. 1990)
Henry’s Law Constant (Pa·m³/mol and reported temperature dependence equations):
1013 (20°C, calculated, Smith et al. 1978)
53.2 (22°C, gas stripping-GC/ECD, Yin & Hassett 1986)
log [H/(atm m³/mol)] = 12.709 – 4711/(T/K), temp range: 8–24°C (gas stripping-GC, Yin & Hassett 1986)
840 (20°C, calculated-P/C, Suntio et al. 1988)
44.1 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 13.899 – 4585/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log K_{OW}:
7.50 (Hansch & Leo 1979)
6.89 (HPLC-RT correlation, Veith et al. 1979; Veith & Kosian 1983)
Bioconcentration Factor, log BCF:

- 2.34, 3.07 (\textit{Gambusia, Physa}, Metcalf et al. 1973)
- 2.78 (\textit{Oedogonium sp.}, Metcalf et al. 1973)
- 2.18 (bioaccumulation factor log BF, adipose tissue in female Albino rats, Ivie et al. 1974)
- -2.02 (milk biotransfer factor log B_{m}, correlated-K_{OW}, Dorough & Ivie 1974)
- 2.34 (fish in static water, Metcalf 1974)
- -1.25 (beef biotransfer factor log B_{b}, correlated-K_{OW}, Bond et al. 1975)
- -1.14 (vegetation, correlated-K_{OW}, De La Cruz & Rajanna 1975)
- 3.86; 3.51; 3.61; 3.70 (\textit{Chlorococcum sp.; Chlamydomonas sp.; Dunaliella tertiolecta; Thallasidsira pseudomana}, Hollister et al. 1975)

- 5.60 (bacterial sorption, Smith et al. 1978)
- 4.26 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980)
- 2.91 (calculated-S, Kenaga 1980)
- 4.71 (fathead minnow to $^{14}$C mirex, Huckins et al. 1982)
- 4.34 (fish, correlated, Mackay 1982)
- 4.26 (fathead minnow, Veith & Kosian 1983)
- 4.09, 3.41 (algae, fish, Verschueren 1983)
- 6.50 (fish, selected, Paterson & Mackay 1985)

1.78–2.87 highest value 2.87 but not equilibrated (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study, Oliver & Niimi 1985)

- > 4.08; 2.87 (rainbow trout, kinetic BCF-k$_{1}$/k$_{2}$; steady-state BCF in laboratory studies, Oliver & Niimi 1985)

6.08; 7.18 (rainbow trout, calculated-K$_{OW}$, Lake Ontario field data, Oliver & Niimi 1985)

- 2.87 (fish, Oliver & Niimi 1985; Oliver 1987)
- 4.34 (worms, Oliver 1987)
- 6.17 (oligochaetes, Connell et al. 1988)
- 6.41 (smelt, Oliver & Niimi 1988)

- 4.31 (\textit{Poecilia reticulata}, Gobas et al. 1989; quoted, Devillers et al. 1996)
- 6.42, 7.16 (guppy, correlated, Gobas et al. 1989)
- 6.40 (Markwell et al. 1989)
- 4.72, 7.07 (dry leaf, wet leaf, Bacci et al. 1990)
- 7.07 (wet leaf, Bacci et al. 1990)
- 5.97, 7.16 (guppy 6.5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor log BAF:

- 8.27 (calculated field bioaccumulation, Thomann 1989)

Sorption Partition Coefficient, log K$_{OC}$:

- 5.56 (natural sediment, Smith et al. 1978)
- 7.38 (av. soils/sediments, Smith et al. 1978)
- 3.76 (soil, quoted exptl., Kenaga 1980)
- 3.08 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 6.00, 5.67 (derived from exptl., calculated-MCI $\chi$, Meylan et al. 1992)
- 6.42 ± 0.39 (suspended particulate matter of the St. Lawrence River, Comba et al. 1993)
- 6.00 (20–25°C, soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 6.00 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
Rate Constants, $k$, and Environmental Half-Lives, $t_{1/2}$:

**Volatilization:** $k = 5.37 \times 10^{-2} \text{ h}^{-1}$ (Hill et al. 1976) with $t_{1/2} = 500 \text{ h}$ from river, $t_{1/2} = 700 \text{ h}$ from pond, $t_{1/2} = 1980 \text{ h}$ from eutrophic lake, and $1 \ t_{1/2} = 980 \text{ h}$ from oligotrophic lake (Smith et al. 1978).

**Photolysis:** rate constants $k < 5.0 \times 10^{-5} \text{ s}^{-1}$ (laboratory data, Smith et al. 1978);
- $k = 4.2 \times 10^{-3} \text{ d}^{-1}$ (field data, Smith et al. 1978);
- $t_{1/2} = 3.9 \times 10^3 \text{ h}$ (aquatic half-life, Haque et al. 1980);
- $k = 0.123 \text{ d}^{-1}$ (sunlight, distilled water containing 2.0 mg DOC/L humic acid, Mudambi & Hassett 1988);
- $k = 0.033 \text{ d}^{-1}$ (sunlight, distilled water, summer, Mudambi & Hassett 1988);
- $k = 0.102 \text{ d}^{-1}$ (sunlight, Lake Ontario water, Mudambi & Hassett 1988);
- $k = 0.019 \text{ d}^{-1}$ (sunlight, distilled water, fall, Mudambi & Hassett 1988).

**Oxidation:** laboratory data $k < 30 \text{ M}^{-1} \text{ s}^{-1}$ (Smith et al. 1978); $t_{1/2} >> 0.7 \text{ yr}$ (Smith et al. 1978; quoted, Cheung 1984).

**Hydrolysis:** laboratory data rate constant $k = 1 \times 10^{-10} \text{ s}^{-1}$ (Smith et al. 1978); $k = 2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 250 \text{ yr}$ (Cheung 1984);
- Degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991).

**Biodegradation:** slow process (Cheung 1984).

**Biotransformation:**

**Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**
- $k_1 > 8.50 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)
- $k_2 < 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)
- $k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ and $k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 78 \text{ d}$ for food concn of 21 ng/g and 145 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for juvenile rainbow trout (Fisk et al. 1998)

**Half-Lives in the Environments:**

**Air:**
- Surface water: overall $t_{1/2} = 0.83 \text{ h}$ in river or stream, $t_{1/2} = 420 \text{ h}$ in pond, and $t_{1/2} = 1480 \text{ h}$ by sorption in both eutrophic lake and oligotrophic lake; with photolysis $t_{1/2} > 8000 \text{ h}$ and oxidation $t_{1/2} > 1000 \text{ h}$ in pond, river, eutrophic lake and oligotrophic lake (Smith et al. 1978);
- Degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991);
- $t_{1/2} = 7 \text{ d}$ in sunlit, air-equilibrated humic acid solution, or natural water (Mudambi & Hassett 1988; Burns et al. 1996).

**Ground water:**
- Soil: estimated field $t_{1/2} = 3000 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- $t_{1/2} = 8.2 \text{ yr}$, extremely persistent in soil (Geyer et al. 2000)

**Biota:**
- $t_{1/2} > 1000 \text{ d}$ (Skene et al. 1981; Oliver & Niimi 1985);
- $t_{1/2} > 28 \text{ d}$ in fathead minnow to $^{14}$C mirex (Huckins et al. 1982);
- $t_{1/2} > 500 \text{ d}$ (4°C, rainbow trout, Niimi & Palazzo 1985);
- $t_{1/2} = 114 \text{ d}$ as observed and $t_{1/2} = 495 \text{ d}$ as adjusted (12°C, rainbow trout, Niimi & Palazzo 1985);
- $t_{1/2} = 103 \text{ d}$ as observed and $t_{1/2} > 1000 \text{ d}$ as adjusted (18°C, rainbow trout, Niimi & Palazzo 1985).

**Depuration $t_{1/2} = 42–78 \text{ d}$ in 30-d uptake and 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)**
18.1.1.61 Monocrotophos

Common Name: Monocrotophos
Synonym: Apadrin, Azodrin, Bilobran, Crotos, ENT 27129, Monocron, Nuvacron
Chemical Name: dimethyl (E)-1-methyl-2-(2-methylcarbamoyl)vinyl phosphate
Uses: systemic insecticide and acaricide to control pests in cotton, sugar cane, coffee, tobacco, olives, rice hops, sorghum, maize, deciduous fruits, citrus fruits, potatoes, sugar beet, tomatoes, soya beans, and ornamentals.
CAS Registry No: 6923-22-4
Molecular Formula: C₇H₁₄NO₅P
Molecular Weight: 223.164
Melting Point (°C):
  55 (Lide 2003)
Boiling Point (°C):
  125 (at 0.0005 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
  1.22 (Tomlin 1994)
Molar Volume (cm³/mol):
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔHₜₘ (kJ/mol):
Entropy of Fusion, ΔSₜₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₘ = 56 J/mol K), F: 0.508 (mp at 55°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  miscible (Spencer 1973; Budavari 1989)
  miscible (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
  9.33 × 10⁻³ (20°C, Eichler 1965)
  9.33 × 10⁻³ (20°C, Wolfdietrich 1965; Melnikov 1971; Budavari 1989)
  9.33 × 10⁻⁴ (20°C, Hartley & Graham-Bryce 1980)
  5.09 × 10⁻³ (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
  2.30 × 10⁻³ (20°C, GC-RT correlation with mp correction, Kim 1985)
  9.00 × 10⁻³ (Hartley & Kidd 1987)
  2.90 × 10⁻⁴ (20°C, Worthing & Hance 1991; Tomlin 1994)
  9.00 × 10⁻³ (20°C, Montgomery 1993)
  0.0295; 0.0039, 0.019 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  2.08 × 10⁻⁶ (20–25°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K₀ₜₚ:
  –1.97 (calculated, Montgomery 1993)
  –0.22 (calculated, Tomlin 1994)
  –0.20 (recommended, Hansch et al. 1995)
Insecticides

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF

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

- 0.0  

- 2.29, 1.65  
  (soil, trans-isomer, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Hydrolysis: calculated $t_{1/2} = 96$ d at pH 5, $t_{1/2} = 66$ d at pH 7 and $t_{1/2} = 17$ d at pH 9 and 20°C (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

- $t_{1/2} = 1–5$ d in laboratory soil (Tomlin 1994).
18.1.1.62 Naled

![Chemical Structure](image)

**Common Name:** Naled  
**Synonym:** Arthodibrom, Dibrom, Bromex, Bromchlophos  
**Chemical Name:** 1,2-dibromo-2,2-dichloroethyl dimethyl phosphate  
**CAS Registry No:** 300-76-5  
**Uses:** insecticide

**Molecular Formula:** C₄H₇Br₂Cl₂O₄P  
**Molecular Weight:** 380.784

**Melting Point (°C):**  
27  
(Lide 2003)

**Boiling Point (°C):**  
110/0.5 mmHg  
(Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

**Density (g/cm³ at 20°C):**  
1.96  
(20°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)  
1.97  
(20°C, Worthing 1987)

**Molar Volume (cm³/mmol):**

**Dissociation Constant, pKₐ:**

**Enthalpy of Vaporization, ∆HV (kJ/mol):**  
77.23  
(Rordorf 1989)

**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:** 0.956 (mp at 27°C)

**Water Solubility (g/m³ or mg/L at 25°C):**  
practically insoluble in water (Hartley & Kidd 1987; Worthing & Walker 1987)  
0.3, 2000  
(quoted, Wauchope et al. 1992)  
2000  
10  
(Montgomery 1993)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
0.266  
(20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)  
6.0 × 10⁻², 0.67, 5.20, 31.0, 150 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
log (P₁/Pa) = 12.307 – 4034.2/(T/K); measured range 50.5–120°C (liquid, gas saturation-GC, Rordorf 1989)  
0.267, 0.00267 (Wauchope et al. 1992)  
0.0267  
0.267  
(20°C, Montgomery 1993)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**

**Octanol/Water Partition Coefficient, log Kₘw:**  
1.38  
(shake flask-GC/UV, Hussain et al. 1974)

**Octanol/Air Partition Coefficient, log Kₐ:**

**Bioconcentration Factor, log BCF or log Kₘi:**
Sorption Partition Coefficient, $\log K_{OC}$:

- 133, 2.26; 2.26 (soil, quoted values; selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

- Volatilization:
  - Photolysis: degraded by sunlight (Tomlin 1994).

- Oxidation:
  - Hydrolysis: completely hydrolyzed in water within 2 d (Windholz 1983; quoted, Montgomery 1993);
    - rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

- Biodegradation:

- Biotransformation:

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

Half-Lives in the Environment:

- Air:
  - Surface water: completely hydrolyzed within 2 d (Windholz 1983; quoted, Montgomery 1993);
    - rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

- Ground water:

- Sediment:

- Soil: field $t_\text{1/2} = 1$ d (Wauchope et al. 1992; Hornsby et al. 1996).

- Biota:
18.1.1.63 Oxamyl

Common Name: Oxamyl
Synonym: D 1410, Dioxamyl, Dupont 1410, Nematicide 1410, Thioxamyl, Vydate
Chemical Name: \(N,N\)-dimethylcarbamoyloxyimino-2-(methylthio)acetamide; ethanimidothioic acid, 2-(dimethylamino)-\(N\)\-[(methylamino)carbonyl]oxy]-2-oxo-methyl ester

Uses: insecticide/acaricide/nematicide
CAS Registry No: 23135-22-0
Molecular Formula: \(\text{C}_7\text{H}_{13}\text{N}_3\text{O}_3\text{S}\)
Molecular Weight: 219.261

Melting Point (°C):
- 109 (Lide 2003)

Boiling Point (°C):
- dec (Lide 2003)

Density (g/cm\(^3\) at 20°C):
- 0.97 (Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm\(^3\)/mol):
- 212.4 (calculated-Le Bas method at normal boiling point)
- 226.1 (calculated-density)

Dissociation Constant, \(pK_a\):

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol): 84

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: 0.150 (mp at 109°C)
- 0.15 (20°C, Suntio et al. 1988)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
- 281000 (Martin & Worthing 1977)
- 282500 (Briggs 1981, Gerstl & Helling 1987)

Vapor Pressure (Pa at 25°C or as indicated):
- 0.0306 (Khan 1980; Spencer 1982)
- 0.0306 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.0311 (Montgomery 1993)
- 0.0310 (Tomlin 1994)

Henry’s Law Constant (Pa·m\(^3\)/mol):
- 0.00026 (calculated-P/C, Suntio et al. 1988)
- 0.260 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, \(\log K_{\text{ow}}\):
- +0.432 (Briggs 1973)
- +0.47 (20–25°C, shake flask-\(^{14}\)C-labeled compound-LSC, Briggs 1981)
- +0.432 (shake flask-centrifuge-liquid scintillation counting method, Gerstl 1984; Gerstl & Helling 1987)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 0.707 (soil, sorption isotherm, converted form reported log $K_{OM}$ of 0.47, Briggs 1981)
- 1.66, 1.07, 1.20, 1.32, 1.84 (5 Israeli soils, organic matter: 0.11% pH 8.5; 0.68% pH 7.9; 0.95% pH 7.8; 1.23% pH 7.2; and 2.03% pH 7.7, reported as $K_{OM}$, batch equilibrium-adsorption isotherms, Gerstl 1984)
- 0.176–1.16, –0.886–0.38 (reported as $K_{OM}$, estimated-S, estimated-$K_{OW}$, Gerstl 1984)
- 0.778 (soil, screening model calculations, Jury et al. 1987b)
- 2.47 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 0.70 (soil, Carsel 1989)
- 1.40 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- –0.70 to 1.40 (Montgomery 1993)
- 1.00 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.06, 1.68 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 1.43, 1.36 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)
- 1.08 (sediment: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

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

Volatilization:
Photolysis: $t_\frac{1}{2}$ = 55.4 h (absorbance wavelength 223 nm) (Montgomery 1993).
Oxidation:
\[ k_{aq.} = (620 \pm 150) \text{M}^{-1} \text{s}^{-1} \] for direct reaction with ozone in water at pH 2–7 and 24 ± 1°C, with a $t_\frac{1}{2}$ = 54 s at pH 7 (Yao & Haag 1991).
Hydrolysis: hydrolysis $t_\frac{1}{2}$ > 31 d at pH 5, 8 d at pH 7 and $t_\frac{1}{2}$ = 3 h at pH 9 (Tomlin 1994).
Biodegradation: decomposition rate constants range from $k$ = 0.182 d$^{-1}$ to 0.021 d$^{-1}$ corresponding to $v$ = 4 to 33 d in Bet Dagan soil depending on moisture, and decomposition rate constant ranges from $k$ = 0.23 to 0.11 d$^{-1}$ corresponding to $t_\frac{1}{2}$ = 3.1 to 6.5 d in five Israeli soils (Gerstl 1984);
$\chi$ = 6 d in screening model calculations (Jury et al. 1987b);
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: measured rate constant $k$ = (620 ± 150) M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2.0–7.0 and 24 ± 1°C, with $t_\frac{1}{2}$ = 54 s at pH 7 (Yao & Haag 1991).
Ground water:
Sediment:
Soil: $t_\frac{1}{2}$ = 9–15 d (Harvey & Han 1978);
$\chi$ = 12–68 d for soils from Holland depending on the moisture content (Smelt et al. 1979);
$\chi$ = 15 d in several soils at 15°C (Bromilow et al. 1980);
decomposition in soil was as a function of moisture content, and followed first-order kinetics with reported
soil $t_\frac{1}{2}$ = 4–13 d at 25°C and, $t_\frac{1}{2}$ = 32.7 d at 15°C, $t_\frac{1}{2}$ = 3.8 d at 35°C in Bet Dagan soil; rate constants
between $k$ = 0.11–0.23 d$^{-1}$ and with $t_\frac{1}{2}$ = 4 d in 5 Israeli soils (Gerstl 1984);
$\chi$ = 6 d in screening model calculations (Jury et al. 1987b);
$\chi$ = 7 d (Worthing & Hance 1991);
$\chi$ = 8–50 d (Ou & Rao 1986) and
$\chi$ = 10.2–13.1, 6.2, 7.1 and 17.8 d in Pitstone, Devizes, Sutton, Veany soils, respectively (Montgomery 1993);
field $t_\frac{1}{2}$ = 4 d (selected, Wauchope et al. 1992; Hornsby et al. 1996).
Biota:
Common Name: Parathion

Chemical Name: $O,O$-diethyl $O$-4-(nitrophenyl) phosphorothioate; diethyl 4-nitrophenyl phosphorothioate; phosphorothioc acid $O,O$-diethyl $O$-(4-nitrophenyl) ester

Uses: insecticide and acaricide to control chewing and sucking insects and mites in fruits, vegetables, ornamentals and field crops.

CAS Registry No: 56-38-2
Molecular Formula: $C_{10}H_{14}NO_5PS$
Molecular Weight: 291.261

Melting Point (°C):

Boiling Point (°C):
115 (at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)
375 (Montgomery 1993; Milne 1995)
105 (at 80 Pa, Tomlin 1994)

Density (g/cm$^3$ at 20°C):
1.26 (25°C, Merck Index 1989; Montgomery 1993)

Molar Volume (cm$^3$/mol):
251.9 (calculated-Le Bas method at normal boiling point)
230.3 (calculated from density)

Dissociation Constant, pK$_a$:
7.14 (Kortum et al. 1961; Wolfe 1980)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
89.92 (Rordorf 1989)

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
19.87 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
24 (Macy 1948; Günther et al. 1968; Melnikov 1971; Spencer 1973)
18–31 (rm temp., > 95% purity with max. particle size 0.07–5.0µ, shake flask-GC, Robeck et al. 1965)
11.9 (20°C, NIEHS 1975; quoted, Freed et al. 1977)
11.9 (20°C, O’Brien 1975)
24 (Martin & Worthing 1977; Worthing & Walker 1987; Hartley & Kidd 1987)
24 (Wauchope 1978; Khan 1980; Lyman 1982; Willis & McDowell 1982)
12.4 (20°C, shake flask-GC, Bowman & Sans 1979, 1983b)
6.54 (shake flask-GC, Felsot & Dahm 1979)
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):

\[
5.04 \times 10^{-3}, 12.3 \times 10^{-3} (20, 30°C, \text{calculated by } \text{Spencer et al. 1979-gas saturation, temp range } 20–45°C, \text{ Bright et al. 1950})
\]

\[
\log (P/\text{mmHg}) = 7.761 – 3395/(T/K); \text{temp range } 25.2–65.5°C (\text{gas saturation, Bright et al. 1950})
\]

\[
2.56 \times 10^{-3} (20°C, \text{effusion, measured range } 25.2–65.5°C, \text{ Williams 1951})
\]

\[
\log (P/\text{mmHg}) = 10.30 – 4400/(T/K); \text{temp range } 25.2–65.5°C (\text{effusion, Williams 1951})
\]

\[
0.76 \times 10^{-3} (20°C, \text{Wolfdietrich 1965})
\]

\[
5.07 \times 10^{-3} (20°C, \text{Spencer 1973})
\]

\[
5.85 \times 10^{-4} (20°C, \text{evaporation rate-gravimetric method gückel et al. 1973, 1974})
\]

\[
0.76 \times 10^{-3} (20°C, \text{gückel et al. 1973, 1974})
\]

\[
1.29 \times 10^{-3} (25°C, \text{gas saturation method, measured range } 25–45°C, \text{Spencer et al. 1979})
\]

\[
\log (P/\text{mmHg}) = 12.66 – 5274/(T/K); \text{temp range } 24.9–45°C (\text{gas saturation Spencer et al. 1979})
\]

\[
6.41 \times 10^{-4} (20°C, \text{evaporation rate, measured range } 20–60°C, \text{gückel et al.1982})
\]

\[
1.29 \times 10^{-3} (\text{Spencer 1983})
\]

\[
1.30 \times 10^{-3} (25.3°C, \text{gas saturation-GC, measured range } 25.3–45°C, \text{Kim et al. 1984; Kim 1985})
\]

\[
\log (P/\text{mmHg}) = 10.5655 – 4645.07/(T/K); \text{temp range } 25.3–45°C (\text{gas saturation, Kim 1985})
\]

\[
0.69 \times 10^{-3} (20°C, \text{extrapolated-Clausius-Clapeyron eq., Kim et al. 1984; Kim 1985})
\]

\[
8.13 \times 10^{-4} (20°C, \text{GC-RT correlation, Kim et al. 1984; Kim 1985})
\]

\[
5.0 \times 10^{-3} (20°C, \text{Hartley & Kidd 1987})
\]

\[
1.80 \times 10^{-3} (25°C, \text{gas saturation-GC, measured range } 25–125°C \text{ Rordorf 1989})
\]

\[
\log (P/P_1) = 13.006 – 4697.2/(T/K); \text{measured range } 32.3–160°C (\text{gas saturation-GC, Rordorf 1989})
\]

\[
6.7 \times 10^{-3} (P_1, \text{GC-RT correlation, Hinckley et al. 1990})
\]

\[
8.90 \times 10^{-4} (20°C, \text{Worthing & Hance 1991; Tomlin 1994})
\]

\[
0.0533 (20°C, \text{Montgomery 1993})
\]

\[
6.67 \times 10^{-4} (20°C, \text{selected, Hornsby et al. 1996})
\]

\[
1.30 \times 10^{-3} (20°C, \text{selected, Siebers & Mattusch 1996})
\]

\[
0.00316; 0.0066, 0.0013, 0.00059, 0.0025 (\text{gradient GC method; quoted lit. values, Tsuzuki 2000})
\]

\[
3.23 \times 10^{-3}; 1.12 \times 10^{-3}, 0.00145 (\text{gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000})
\]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):

\[
0.120 (20°C, \text{calculated-P/C, Mackay & Shiu 1981})
\]

\[
0.074 (20°C, \text{volatilization rate, Burkhard & Guth 1981})
\]

\[
0.096 (24°C, \text{calculated-P/C, Chiou et al. 1980})
\]

\[
0.015 (\text{calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989})
\]

\[
0.012 (20°C, \text{calculated-P/C, Suntio et al. 1988})
\]

\[
0.015 (\text{calculated-P/C, Taylor & Glotfelty 1988})
\]

\[
0.0087 (23°C, \text{Fendinger & Glotfelty 1990})
\]

\[
0.057 (\text{calculated-P/C, Howard 1991})
\]

\[
0.030 (\text{calculated-bond contribution method, Meylan Howard 1991})
\]

\[
0.0087 (\text{calculated-P/C, Montgomery 1993})
\]

\[
0.020 (\text{selected, Siebers & Mattusch 1996})
\]

Octanol/Water Partition Coefficient, log \(K_{OW}\):

\[
3.81 (\text{shake flask-GC, Chiou et al. 1977; Freed et al. 1977})
\]

\[
3.40 (\text{shake flask-LSC, Felsot & Dahm 1979})
\]

\[
3.81 (\text{shake flask-GC, Freed et al. 1979})
\]
3.80 (Hansch & Leo 1979)
3.93 (shake flask-UV, Lord et al. 1980)
3.93 (shake flask-GC, Briggs 1981)
3.76 (shake flask-GC, Bowman & Sans 1983b)
3.83 (Hansch & Leo 1985)
2.15–3.93 (Montgomery 1993)
3.83 (recommended, Sangster 1993)
3.83 (Tomlin 1994)
3.83 (recommended, Hansch et al. 1995)
3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)
4.32 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.53 (fish in static water, Metcalf & Sanborn 1975)
1.81 (tadpoles, Hall & Kolbe 1980)
2.00, 2.54 (calculated-S, K\text{OC}, Kenaga 1980)
3.14 (earthworms, Lord et al. 1980)
4.00 (log BCF\text{liquid}, Briggs 1981)
2.68 (calculated-K\text{OM}, Hansch & Leo 1985)
2.48 (Am. oysters after 84 d.; Howard 1991)
1.48, 2.34 (av., fathead minnow after 70 d, 820,138 d, Howard 1991)
2.34 (av., fathead minnow after 82–138 d, Howard 1991)
1.91, 2.27, 2.40, 1.43 (av., bluegill after 12 h, 29 h, 46 h, 504 d, Howard 1991)
1.95, 2.39, 2.50 (average, brook trout muscle after 8 h, 6 d, 180 d, Howard 1991)
1.90 (Isnard & Lambert 1988)
2.53 (Pait et al. 1992)

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

3.68 (soil, Swoboda & Thomas 1968; quoted, Kenaga 1980; Kenaga & Goring 1980)
4.02 (average, 4 soils, Hamaker & Thompson 1972)
3.30 (average, soils, Chiou et al. 1979)
2.88 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.90 (calculated-S, Mill et al. 1980)
4.03 (average soils/sediments, Rao & Davidson 1980)
3.02 (soil, sorption isotherm, converted from the reported log K\text{OM} of 2.78, Briggs 1981)
3.25, 3.95, 3.42 (estimated-S, calculated-S and mp, calculated-K\text{OM}, Karickhoff 1981)
2.26–3.96 (reported as log K\text{OM}, Minkelgrin & Gerstl 1983)
2.83 (average, 8 Israeli soils, Gerstl & Minkelgrin 1984)
3.19 (average, 4 Israeli sediments, Gerstl & Minkelgrin 1984)
3.52, 2.58 (quoted, calculated-MCI \chi, Gerstl & Helling 1987)
3.04 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
3.68, 3.33 (reported, estimated as log K\text{OM}, Magee 1991)
3.15 (estimated-QSAR and SPARC, Kollig 1993)
2.50–4.20 (Montgomery 1993)
3.70 (20°C, selected, Hornsby et al. 1996)
3.20 (soil, calculated-MCI \chi, Sabljic et al. 1995)
3.05, 3.09, 2.94 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, average, Delle Site 2001)
3.17, 3.09 (average values for sediments with OC \geq 0.5%, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:

Volatilization: expl. t_1/2 = 14 d in nonstirred aqueous solutions and t_1/2 = 9.3 d in stirred aqueous solutions, and estimated t_1/2 ~ 13 d in nonstirred aqueous solutions and t_1/2 ~ 8.7 d in stirred aqueous solutions (Chiou et al. 1980).
Photolysis: photo-reacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlozhauer 1983)

direct photolysis has a $t_{1/2} < 1$ d to 10 d in surface waters, the presence of photosensitizers, free radicals, hydrogen peroxide, or algae which are found in eutrophic waters may accelerate degradation considerably (GEMS 1986; quoted, Howard 1991)

photodegradation $t_{1/2} = 88$ h (Hazardous Substances Data Bank 1989; quoted, Montgomery 1993)

t$_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and $t_{1/2} = 9$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (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: $k_{OH(calc)} = 92 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Winer & Atkinson 1990).

Hydrolysis:

$k(second-order alkaline) = 1.2 \times 10^{-3}$ M$^{-1}$ s$^{-1}$ at 27°C (Ketelaar 1950; quoted, Wolfe 1980)

$t_{1/2} = 130$ d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979; Montgomery 1993)

$t_{1/2} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C, respectively, in estuarine water with salinity of 25.7% at pH 7.8, and $t_{1/2}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

t$_{1/2} = 24$ wk at pH 6, $t_{1/2} = 19$ wk at pH 7.4 and 20°C (Freed et al. 1979; quoted, Howard 1991; Montgomery 1993)

$t_{1/2} = 43$ wk at pH 5, $t_{1/2} = 24$ wk at pH 6, and $t_{1/2} = 15$ wk at pH 8 and 20°C (Chapman & Cole 1982; quoted, Howard 1991; Montgomery 1993)

$k(alkaline) = 2.3 \times 10^{-2}$ M$^{-1}$ s$^{-1}$, $k(neutral) = 4.5 \times 10^{-8}$ s$^{-1}$ in aqueous buffer at 20°C (Harris 1982)

$k = 2.4 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993); $t_{1/2} = 3.5$ wk at pH 6 (Montgomery 1993)

$t_{1/2} = 272$ d at pH 4, $t_{1/2} = 260$ d at pH 7, and $t_{1/2} = 130$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: generally occurs with a half-life of several weeks but in well acclimated water, complete degradation may occur in two weeks (Eichelberger & Lichtenberg 1971; Sharom et al. 1980; quoted, Howard 1991)

$t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$k = 0.029$ d$^{-1}$ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982)

$t_{1/2} = 18$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

$k < 0.00016$ d$^{-1}$ of aerobic degradation observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971)
$t_{1/2} = 3670$ h at pH 5 and $t_{1/2} = 523$ h at pH 9 in water at 20°C (Gomaa & Faust 1972)

estimated $t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$t_{1/2} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C, respectively, in estuarine water with salinity of 25.7% at pH 7.8, and $t_{1/2}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

$t_{1/2} = 7.84$ d in the Indian River water at 24 ppt salinity; pH 8.16 (Wang & Hoffman 1991);

photolysis $t_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and 9 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994);

$t_{1/2} = 120$ d at 6°C, $t_{1/2} = 84$ d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 120$ d at 6°C, $t_{1/2} = 86$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 122$ d at 6°C, $t_{1/2} = 33$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 542$ d at 6°C, $t_{1/2} = 44$ d at 22°C in darkness, $t_{1/2} = 18$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).
Ground water:
Sediment:
Soil: persistence of one week (Edwards 1973; quoted, Morrill et al. 1982);
persistence of less than one month (Wauchope 1978);
$t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 1.5$ wk in nonsterile organic soil (Miles et al. 1979);
estimated first-order $t_{1/2} = 23.9$ d from biodegradation rate constant $k = 0.029$ d$^{-1}$ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982);
moderately persistent in soil with $t_{1/2} = 20–100$ d (Willis & McDowell 1982);
reported $t_{1/2} = 18$ d calculated using screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
av. degradation rate constant $k = 0.030$ d$^{-1}$ in silty clay with $t_{1/2} = 23$ d and av. degradation rate constant $k = 0.0315$ d$^{-1}$ in sandy clay with $t_{1/2} = 22$ d (Sattar 1990);
field $t_{1/2} = 14$ d (selected, Halfon et al. 1996);
soil $t_{1/2} = 6$ d (Pait et al. 1992)
Biota: biochemical $t_{1/2} = 15$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

### TABLE 18.1.1.64.1

**Reported vapor pressures of parathion 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>20</td>
<td>5.04 × 10^{-3}</td>
<td>20</td>
<td>2.61 × 10^{-3}</td>
<td>25</td>
<td>1.29 × 10^{-3}</td>
<td>20</td>
<td>6.41 × 10^{-4}</td>
</tr>
<tr>
<td>25</td>
<td>7.96 × 10^{-3}</td>
<td>25.4</td>
<td>4.68 × 10^{-3}</td>
<td>35</td>
<td>4.32 × 10^{-3}</td>
<td>40</td>
<td>7.29 × 10^{-3}</td>
</tr>
<tr>
<td>30</td>
<td>1.23 × 10^{-2}</td>
<td>54.5</td>
<td>0.088</td>
<td>45</td>
<td>0.01680</td>
<td>45</td>
<td>0.01680</td>
</tr>
<tr>
<td>35</td>
<td>1.86 × 10^{-2}</td>
<td>70.7</td>
<td>0.373</td>
<td>45</td>
<td>0.01680</td>
<td>60</td>
<td>6.10 × 10^{-2}</td>
</tr>
<tr>
<td>40</td>
<td>2.79 × 10^{-2}</td>
<td>100</td>
<td>2.866</td>
<td>45</td>
<td>0.01680</td>
<td>60</td>
<td>6.10 × 10^{-2}</td>
</tr>
<tr>
<td>45</td>
<td>0.04135</td>
<td>140</td>
<td>58.66</td>
<td>140</td>
<td>142.7</td>
<td>25</td>
<td>1.26 × 10^{-3}</td>
</tr>
<tr>
<td>45</td>
<td>0.04135</td>
<td>140</td>
<td>58.66</td>
<td>140</td>
<td>142.7</td>
<td>25</td>
<td>1.26 × 10^{-3}</td>
</tr>
</tbody>
</table>

**1.**

<table>
<thead>
<tr>
<th>Bright et al. 1950</th>
<th>Williams 1951</th>
<th>Spencer et al. 1979</th>
<th>Gückel et al. 1982</th>
</tr>
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<td><strong>Gas saturation</strong></td>
<td><strong>Dynamic/microdistillation</strong></td>
<td><strong>Gas saturation-GC</strong></td>
<td><strong>Evaporation rate</strong></td>
</tr>
<tr>
<td>T/°C</td>
<td>P/mmHg</td>
<td>T/°C</td>
<td>P/mmHg</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>20</td>
<td>5.04 × 10^{-3}</td>
<td>20</td>
<td>2.61 × 10^{-3}</td>
</tr>
<tr>
<td>25</td>
<td>7.96 × 10^{-3}</td>
<td>25.4</td>
<td>4.68 × 10^{-3}</td>
</tr>
<tr>
<td>30</td>
<td>1.23 × 10^{-2}</td>
<td>54.5</td>
<td>0.088</td>
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<tr>
<td>35</td>
<td>1.86 × 10^{-2}</td>
<td>70.7</td>
<td>0.373</td>
</tr>
</tbody>
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TABLE 18.1.1.64.1 (Continued)

2.

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<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
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<tr>
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<td>0.00131</td>
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<td>34.9</td>
<td>0.00409</td>
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<td>45.0</td>
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<table>
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<th>eq. 1</th>
<th>P/mmHg</th>
<th>eq. 1</th>
<th>P/Pa</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>10.5654</td>
<td>A</td>
<td>13.006</td>
</tr>
<tr>
<td>B</td>
<td>4645.07</td>
<td>B</td>
<td>4697.2</td>
</tr>
</tbody>
</table>

FIGURE 18.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for parathion.
18.1.1.65 Parathion-methyl

Common Name: Parathion-methyl
Synonym: Bladan M, Folidol-M, Metacide, Nitox 80
Chemical Name: \(O,O\)-dimethyl \(O-4\)-(nitrophenyl) phosphorothioate; dimethyl 4-nitrophenyl phosphorothioate
Uses: insecticide to control chewing and sucking insects, and mites in a wide range of crops, including fruits, vines, vegetables, ornamentals, cotton, and also used as acaricide.
CAS Registry No: 298-00-0
Molecular Formula: \(C_8H_{10}NO_5PS\)
Molecular Weight: 263.208
Melting Point (°C):
- 38 (Lide 2003)
Boiling Point (°C):
- 109 (at 0.05 mmHg, Freed et al. 1977)
- 119 (at 0.1 mmHg, Hartley & Kidd 1987)
- 154 (at 1.0 mmHg, Hartley & Kidd 1987; Tomlin 1994)
- 143 (Howard 1991)
Density (g/cm\(^3\) at 20°C):
- 1.358 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Molar Volume (cm\(^3\)/mol):
- 207.5 (calculated-Le Bas method at normal boiling point)
- 194.0 (calculated from density)
Dissociation Constant, \(pK_a\):
- 7.15 (Kortum et al. 1961; Wolfe 1980)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
- 24.06 (Plato & Glasgow 1969)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), \(F\): 0.746 (mp at 38°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
- 55 (Melnikov 1971)
- 60 (Leonard et al. 1976; Khan 1980)
- 57 (Martin & Worthing 1977)
- 50 (Smith et al. 1978; Wauchope 1978)
- 37.7 (19.5°C, shake flask-GC, Bowman & Sans 1979, 1983b)
- 55 (20°C, Freed et al. 1979)
- 60 (Khan 1980)
- 53 (Weber et al. 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):
- 0.00133 (20°C, Wolfdietrich 1965; von Rümker & Horay 1972)
- 0.00129 (20°C, Gückel et al. 1973)
- 0.0023 (Grover et al. 1976)
- 0.00229* (24.9°C, gas saturation-GC, measured range 24.9–45.1°C, Spencer et al. 1979)
\[\log (P/\text{mmHg}) = 14.37 - 3700/(T/K);\text{ temp range }24.9-34.9°C\text{ (gas saturation, Spencer et al. 1979)}\]
\[\log (P/\text{mmHg}) = 10.61 - 4543/(T/K);\text{ above mp }35.2–35.4°C\text{ (gas saturation, Spencer et al. 1979)}\]
Insecticides

0.0013 (Worthing 1979)
> 0.0133 (20–25°C, Weber et al. 1980)
0.0020* (gas saturation-GC, measured range 25.4–45.1°C, Kim et al. 1984)
log (P/mmHg) = 9.0935 – 4063.65/(T/K); temp range 25.4–45°C (gas saturation method, Kim et al. 1984)
0.00084 (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)
log (P/mmHg) = 17.0502 – 6520.21/(T/K); temp range 25.4–34.3°C (gas saturation, Kim 1985)
0.0013 (20°C, Hartley & Kidd 1987)
0.0015 (22°C, selected, Seiber et al. 1989)
0.023 (GC-RT correlation, supercooled liquid P, Hinckley et al. 1990)
0.0024 (selected, Taylor & Spencer 1990)
0.0002 (20°C, Worthing & Hance 1991; Tomlin 1994)
0.002 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00041 (Tomlin 1994)
0.00955 (gradient GC method; Tsuzuki 2000)
9.77 × 10^–3; 4.90 × 10^–3, 0.00389 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)

Henry’s Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0101 (Metcalf et al. 1980)
0.0061 (estimated, Metcalf et al. 1980)
0.0109 (calculated-P/C, Jury et al. 1987a; Jury & Ghodrati 1989)
0.021 (20°C, calculated-P/C, Suntio et al. 1988)
0.0101 (22°C, selected, Seiber et al. 1989)
0.0062 (wetted wall column method-GC, Fendinger & Glotfelty 1990)
0.0170 (calculated-bond contribution method, Meylan & Howard 1991)
0.0062 (23°C, quoted, Schomburg et al. 1991)
0.00383 (20°C, wetted wall column-GC, Rice et al. 1997b)

Octanol/Water Partition Coefficient, log K_{ow}:
2.04 (shake flask-GC, Jaglan & Gunther 1970)
2.04 (shake flask, Leo et al. 1971)
2.99 (shake flask, Mundy et al.1978)
2.68 (shake flask-HPLC, Moody et al.1987)
3.32 (Hansch & Leo 1979)
3.32 (Rao & Davidson 1980)
2.94 (shake flask-GC, Bowman & Sans 1983b)
1.80 (shake flask-GC, Schimmel et al. 1983)
2.86 (Hansch & Leo 1985)
2.86 (recommended, Sangster 1993)
2.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.00 (Tomlin 1994)
2.86 (recommended, Hansch et al. 1995)
2.71 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
0.778, 0.0 (carp/lipids, carp/muscle, Chigareva 1973)
1.98 (fish in static water, Metcalf 1974)
2.69 (bacteria, Smith et al. 1978)
1.80, 2.89 (calculated-S; calculated-K_{oc}, Kenaga 1980)
3.039 ± 0.005 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
2.98 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
3.04 (Poecilia reticulata, De Bruijn & Hermens 1991)
1.85 (Pait et al. 1992)
1.92 (paddy field fish, Tejada 1995)
Sorption Partition Coefficient, log $K_{OC}$:

3.99 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
1.699 (av. all sediments, Smith et al. 1978)
2.63 (av. of 3 soils, Rao & Davidson 1979)
2.67 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.71 (Rao & Davidson 1980)
3.02, 3.47, 2.93 (estimated-S, S and mp, $K_{mp}$, Karickhoff 1981)
3.71 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
3.84, 1.97 (quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
3.00 (soil, calculated-MCI 1$\chi$, Sabljic et al. 1995)
2.68 (sediment, estimated, Paraiba et al. 1999)
3.27, 2.84 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.82, 2.74 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

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

Volatilization: volatilization rate $k < 0.01$ kg ha$^{-1}$ d$^{-1}$ in a flooded rice field (Seiber et al. 1986; Seiber & McChesney 1987; quoted, Seiber et al. 1989)

Photolysis: lab. rate constant $k = 2.7 \times 10^{-7}$ s$^{-1}$ in early January with photolysis $t_{1/2} = 240$ h, 850 h, 850 h and 170 h in river, pond, eutrophic lake and oligotrophic lake predicted by the one-compartment model (Smith et al. 1978; quoted, Howard et al. 1991);

$\psi_{H_2O} = 8$ d in summer and $t_{1/2} = 38$ d in winter for direct sunlight photolysis in natural water (Smith et al. 1978; quoted, Howard 1991; Howard et al. 1991);

photolytic $t_{1/2} = 200$ h in aquatics (Haque et al. 1980);

photoreacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlotzhauer 1983).

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:

$k = 3.0$ M$^{-1}$ s$^{-1}$ (Smith et al. 1978)

photooxidation half-life of 3.6 d for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1991);

photooxidation half-life of 1.0–10.5 h based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

$k = 4 \times 10^{-2}$ mol min$^{-1}$ with $t_{1/2} = 125$ h for pH $<11.0$ at 15°C (Ketelaar & Gersmann 1958; quoted, Freed 1976)

$k = 1.1 \times 10^{-5}$ s$^{-1}$ with a half-life of 8.4 h at pH 6 buffer at 70°C in 20% ethanol aqueous solution (Ruzicka et al. 1967; quoted, Freed 1976; Smith et al. 1978)

$\psi_{H_2O} = 1.7$ wk at pH about 6 and room temp. (Cowart et al. 1971; quoted, Smith et al. 1978)

$k = 1.1 \times 10^{-7}$ s$^{-1}$ with $t_{1/2} = 72$ d at pH 7 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991)

$k = 9 \times 10^{-7}$ s$^{-1}$ (Smith et al. 1978)

$k(alkaline) = 5.3 \times 10^{-3}$ M$^{-1}$ s$^{-1}$ at 27°C and pH 10 (Smith et al. 1978; quoted, Wolfe 1980)

$\psi_{H_2O} = 68$ d at pH 5, $\psi_{H_2O} = 40$ d at pH 7, $\psi_{H_2O} = 33$ d at pH 9 at 25°C (Tomlin 1994).

Biodegradation:

$k = 1.7 \times 10^{-7}$ g cell$^{-1}$ h$^{-1}$ (Smith et al. 1978);

$\psi_{aq}(aerobic) = 360–1680$ h, based on an unacclimated aerobic river die-away test data (Bourquin et al. 1979; Spain et al. 1980; quoted, Howard et al. 1991);

$\psi_{aq}(anaerobic) = 24–168$ h, based on unacclimated anaerobic soil and sediment grab sample data (Adhya et al. 1981; Wolfe et al. 1986; quoted, Howard et al. 1991);

$\psi_{s} = 15$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1987a, b; Jury & Ghodrati 1989);

$k = (0.003 \pm 0.0003)$ h$^{-1}$ with half-life of 220.9 h in surface aerobic soils at Williamsburg,

$k = (0.0017 \pm 0.00009)$ h$^{-1}$ with half-life of 410 h in subsurface aerobic soils at Sault Ste. Marie (Ward 1985)

$k = 0.30$ d$^{-1}$ in river sediment, $k = 0.02$ d$^{-1}$ in river water (Cripe et al. 1987; quoted, Battersby 1990)
Insecticides

Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

\[ k_1 = (2.59 \pm 0.88) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1} \text{ (guppy, De Bruijn & Hermens 1991)} \]

\[ k_2 = (2.38 \pm 0.14) \text{ d}^{-1} \text{ (guppy, De Bruijn & Hermens 1991)} \]

\[ k_2 = 1.71 \text{ d}^{-1} \text{ (guppy, calculated-KOW, De Bruijn & Hermens 1991)} \]

\[ k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)} \]

\[ k_2 = (0.11 \pm 0.03) \times 10^{-3} \text{ (GSH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)} \]

Half-Lives in the Environment:
Air: estimated \( t_{\text{1/2}} = 3.6 \text{ d} \) for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1991);

photooxidation \( t_{\text{1/2}} = 1.0-10.5 \text{ h} \) in air based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

reaction rate \( k = 4.77 \times 10^{-4} \text{ min}^{-1} \) in air (Paraiba et al. 1999).

Surface water: persistence up to 4.0 wk in river water (Eichelberger & Lichtenberg 1971);

overall \( t_{\text{1/2}} = 0.6 \text{ h} \) in river, \( t_{\text{1/2}} = 15 \text{ h} \) in eutrophic pond, \( t_{\text{1/2}} = 28.3 \text{ h} \) in eutrophic lake and \( t_{\text{1/2}} = 157.5 \text{ h} \) oligotrophic lake (Smith et al. 1978);

\( t_{\text{1/2}} = 8 \text{ d} \) in summer and \( t_{\text{1/2}} = 38 \text{ d} \) in winter for direct sunlight photolysis in natural water (Howard et al. 1991); Schimmel et al. 1983); first-order biodegradation rate constant \( k = 0.30 \text{ d}^{-1} \) in river sediment and \( k = 0.02 \text{ d}^{-1} \) in river water (Cripe et al. 1987; quoted, Battersby 1990);

\( t_{\text{1/2}} = 44 \text{ h} \) of dissipation from rice field water (Seiber & McChesney 1987; quoted, Seiber et al. 1989)

\( t_{\text{1/2}} = 237 \text{ d} \) at 6°C, 46 d at 22°C in darkness for Milli-Q water at pH 6.1; \( t_{\text{1/2}} = 95 \text{ d} \) at 0°C, 23 d at 22°C in darkness, \( t_{\text{1/2}} = 11 \text{ d} \) under sunlight conditions for river water at pH 7.3; \( t_{\text{1/2}} = 173 \text{ d} \) at 6°C, \( t_{\text{1/2}} = 18 \text{ d} \) at 22°C in darkness for filtered river water at pH 7.3; \( t_{\text{1/2}} = 233 \text{ d} \) at 6°C, \( t_{\text{1/2}} = 30 \text{ d} \) at 22°C in darkness, \( v = 34 \text{ d} \) under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

reaction rate \( k = 3.80 \times 10^{-4} \text{ min}^{-1} \) in water (Paraiba et al. 1999).

Ground water: \( t_{\text{1/2}} = 24-1680 \text{ h} \) based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: \( t_{\text{1/2}} < 1.2 \text{ d} \) in 10 g sediment/100 mL pesticide-seawater solution under untreated conditions and \( t_{\text{1/2}} > 28 \text{ d} \) under sterile conditions (Schimmel et al. 1983); disappearance rate constants:

\( k = (3.5 \pm 0.6) \times 10^{-3} \text{ min}^{-1} \) in Beaver Dam sediments samples at pH 6.7, \( k = (2.9 \pm 1.2) \times 10^{-3} \text{ min}^{-1} \) in Memorial Park sediments samples at pH 6.5 and \( k = (2.8 \pm 2.4) \times 10^{-3} \text{ min}^{-1} \) in Hickory Hills sediments samples at pH 6.9 near Athens, Georgia (Wolfe et al. 1986);

reaction rate \( k = 2.85 \times 10^{-5} \text{ min}^{-1} \) in sediment (Paraiba et al. 1999).

Soil: \( t_{\text{1/2}} = 2,408,640 \text{ h} \) based on unacclimated aerobic soil grab sample data (Davidson et al. 1980; Butler et al. 1981; quoted, Howard et al. 1991); measured dissipation rate \( k = 0.010-0.034 \text{ d}^{-1} \) (Baker & Applegate 1970; quoted, Nash 1988); estimated dissipation rate \( k = 0.029, 0.042 \text{ d}^{-1} \) (Nash 1988); persistence of less than one month (Wauchope 1978); non-persistent in soils with \( t_{\text{1/2}} < 20 \text{ d} \) (Willis & McDowell 1982);

rate constant \( k = 0.16 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 4 \text{ d} \) under laboratory conditions and rate constant \( k = 0.046 \text{ d}^{-1} \) with \( t_{\text{1/2}} = 15 \text{ d} \) under field conditions (Rao & Davidson 1980);

\( t_{\text{1/2}} = 5.0 \text{ d} \) (Wauchope et al. 1992; quoted, Halton et al. 1996; Hornsby et al. 1996); soil \( t_{\text{1/2}} = 44 \text{ d} \) (Pait et al. 1992).

Biota: biochemical \( t_{\text{1/2}} = 15 \text{ d} \) from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).
TABLE 18.1.1.65.1
Reported vapor pressures of parathion-methyl at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\end{align*}
\]

\[
\begin{align*}
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2a)
\end{align*}
\]

Spencer et al. 1979

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.9</td>
<td>0.00229</td>
</tr>
<tr>
<td>30.0</td>
<td>0.00529</td>
</tr>
<tr>
<td>34.9</td>
<td>0.00960</td>
</tr>
<tr>
<td>38.6</td>
<td>0.0148</td>
</tr>
<tr>
<td>39.7</td>
<td>0.0164</td>
</tr>
<tr>
<td>41.7</td>
<td>0.0207</td>
</tr>
<tr>
<td>45.1</td>
<td>0.0291</td>
</tr>
</tbody>
</table>

Kim et al. 1984

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.4</td>
<td>0.00205</td>
</tr>
<tr>
<td>30.1</td>
<td>0.00489</td>
</tr>
<tr>
<td>34.3</td>
<td>0.00879</td>
</tr>
<tr>
<td>38.5</td>
<td>0.0150</td>
</tr>
<tr>
<td>41.7</td>
<td>0.0202</td>
</tr>
<tr>
<td>45.1</td>
<td>0.0278</td>
</tr>
<tr>
<td>20</td>
<td>0.00084#</td>
</tr>
<tr>
<td>25</td>
<td>0.0020#</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\text{mp/°C} &= 34.6 \\
\Delta H_v &= 109.2 \text{ kJ/mol}
\end{align*}
\]

above the melting point

\[
\begin{align*}
\text{eq. 1} &= \text{P/mmHg} \\
A &= 14.37 \\
B &= 5700
\end{align*}
\]

\[
\begin{align*}
\text{eq. 1} &= \text{P/mmHg} \\
A &= 9.9035 \\
B &= 4063.65
\end{align*}
\]

\[
\Delta H_v = 87.03 \text{ kJ/mol}
\]

FIGURE 18.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for parathion-methyl.
18.1.1.66 Pentachlorophenol

(See also chapter 14. Phenolic Compounds)

Common Name: Pentachlorophenol
Synonym: chlorophen, PCP, penchlorol
Chemical Name: pentachlorophenol
Uses: insecticide/fungicide/herbicide; control of termites; as wood preservatives to protect against fungal rots and wood boring insects; as a pre-harvest defoliant in cotton; and also as a general pre-emergence herbicide.
CAS Registry No: 87-86-5
Molecular Formula: C₆Cl₅OH
Molecular Weight: 266.336

Melting Point (°C):
191 (Firestone 1977; Weast 1982–83; Hartley & Kidd 1987)
187 (Schmidt-Bleek et al. 1982)
174 (Lide 2003)

Boiling Point (°C):
310 (Verschueren 1977, 1983; Callahan et al. 1979)
309–310 (Hartley & Kidd 1987)
310 (dec, Lide 2003)

Density (20°C, g/cm³):
1.987 (Firestone 1977)
1.978 (Schmidt-Bleek et al. 1982; Verschueren 1983)
1.980 (22°C, Hartley & Kidd 1987)

Dissociation Constant, pKₐ:
4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)
5.0 (Farquharson et al. 1958; Renner 1990)
4.92 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)
4.71 (Cessna & Grover 1978; Saarikoski & Vilukseta 1982; Saarikoski et al. 1986; Tratnyek & Hoigné 1991)
5.30 (Gebeffügi et al. 1979; Xie 1983; Schellenberg et al. 1984)
4.70 (Crosby 1981; Hoigné & Bader 1983)
5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)
4.90 (Xie & Dryssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)
4.75 (Leuenberger et al. 1985)
4.60 (Nendza & Seydel 1988)

Molar Volume (cm³/mol):
207.9 (calculated-Le Bas method at normal boiling point)
134.3 (calculated-density)

Enthalpy of Fusion, ΔH₉₀ (kJ/mol):
17.154 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS₉₀ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS₉₀ = 56 J/mol K) F: 0.0345 (mp at 174°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
15.4 (gravimetric, Carswell & Nason 1938)
18 (27°C, gravimetric, Carswell & Nason 1938)
9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)
<table>
<thead>
<tr>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>(20°C, shake flask-UV, at pH 3.0, Bevenue &amp; Beckman 1967)</td>
</tr>
<tr>
<td>10</td>
<td>(shake flask-gravimetric, at pH 5.0, Toyota &amp; Kuwahara 1967)</td>
</tr>
<tr>
<td>14</td>
<td>(gravimetric at pH 5.0, Toyota &amp; Kuwahara 1967)</td>
</tr>
<tr>
<td>20–25</td>
<td>(selected, Günther et al. 1968;)</td>
</tr>
<tr>
<td>20</td>
<td>(30°C, Firestone 1977)</td>
</tr>
<tr>
<td>14</td>
<td>(20°C, Verschueren 1977, 1983)</td>
</tr>
<tr>
<td>20</td>
<td>(20°C, Körte et al. 1978)</td>
</tr>
<tr>
<td>14</td>
<td>(Kenaga &amp; Goring 1980; Geyer et al. 1982; McKim et al. 1985)</td>
</tr>
<tr>
<td>15</td>
<td>(23°C, Klöpffer et al. 1982)</td>
</tr>
<tr>
<td>20</td>
<td>(20°C, Schmidt-Bleek et al. 1982)</td>
</tr>
<tr>
<td>5–10</td>
<td>(at pH 5–6 in contaminated water, Goerlitz et al. 1985)</td>
</tr>
<tr>
<td>14</td>
<td>(recommended at pH 4.5–5.5, IUPAC 1985)</td>
</tr>
<tr>
<td>80</td>
<td>(20°C, Hartley &amp; Kidd 1987)</td>
</tr>
<tr>
<td>41</td>
<td>(predicted-MCI $\chi$, Nirmalakhandan &amp; Speece 1988)</td>
</tr>
<tr>
<td>8 ± 2</td>
<td>(shake flask-UV at pH 2.5, Valsaraj et al. 1991)</td>
</tr>
<tr>
<td>32 ± 3</td>
<td>(shake flask-UV at pH 5.0, Valsaraj et al. 1991)</td>
</tr>
<tr>
<td>19</td>
<td>(quoted, Müller &amp; Klein 1992)</td>
</tr>
<tr>
<td>18.4</td>
<td>(shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)</td>
</tr>
</tbody>
</table>

**Vapor Pressure (Pa at 25°C or as indicated):**

- 0.0227 (20°C, static method, Carswell & Nason 1938)
- 0.0147 (20°C, Bevenue & Beckman 1967)
- 0.231 (supercooled liq. extrapolated-Antoine eq., Weast 1976–77)
- 0.10 (Weast 1972–73)
- 0.0211 (Chiou & Freed 1977)
- 0.0213 (Firestone 1977)
- 0.0147–0.0227 (20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
- 0.0956 (supercooled liquid, Hamilton 1980; quoted, Bidleman & Renberg 1985)
- 0.00415 (23°C, OECD, Klöpffer et al. 1982)
- 0.0093 (20°C, Schmidt-Bleek et al. 1982)
- 0.0147 (20°C, Verschueren 1983; Howard 1991)
- 0.1153 (extrapolated-Antoine eq., Boublik et al. 1984)
- 0.50 (20°C, quoted, Crossland & Wolff 1985)
- 0.115 (capillary GC-RT correlation, Bidleman & Renberg 1985)
- 0.127 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

**Henry’s Law Constant (Pa m³/mol):**

- 0.00248 (calculated-P/C, Hellmann 1987)
- 0.0127 (estimated-bond contribution, Hellmann 1987)
- 0.277 (calculated-P/C, Howard 1991)
- 0.079 (calculated-P/C, this work)

**Octanol/Water Partition Coefficient, log $K_{OW}$:**

- 5.01 (quoted unpublished result, Leo et al. 1971)
- 5.01 (Firestone 1977)
- 5.01, 5.12, 5.86, 3.81 (Hansch & Leo 1979)
- 5.01 (calculated, Veith et al. 1979b; McLeeese et al. 1979)
- 2.97 (Veith et al. 1979)
- 3.69 (quoted from Kotzias 1980 unpublished result, Geyer et al. 1982)
- 4.16 (Rao & Davidson 1980)
- 5.10 (calculated-HPLC-k’ correlation, Butte et al. 1981)
- 4.00, 0.0 (at pH 4, 8, Renberg 1981)
- 5.08 (RP-HPLC-k’ correlation, Miyake & Terada 1982)
Insecticides

5.15 (shake flask-GC, Saarikoski & Viluksela 1982; Saarikoski et al. 1986)
5.05 (Kaiser & Valdmanis 1982)
4.84 (shake flask-GC, apparent value at pH 1.2, Kaiser & Valdmanis 1982)
1.30 (shake flask-GC, apparent value at pH 10.5, Kaiser & Valdmanis 1982)
3.69 (Geyer et al. 1982, Schmidt-Bleek et al. 1982)
3.29 (shake flask average, OECD/EEC Lab. comparison tests, Harnisch et al. 1983)
5.01 (Verschueren 1983)
5.85 (calculated as per Leo et al. 1971, Xie 1983)
5.05 ± 0.07 (exptl.-ALPM, Garst & Wilson 1984)
5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
5.04, 5.08, 5.85, 5.22 (shake flask-GC, HPLC-k’, calculated-π const., calculated-f const., Xie et al. 1984; Bintein & Devillers 1994)
5.05 (calculated, Xie & Dryssen 1984; quoted, Lagas 1988)
4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
2.50 (at pH 4.7, Geyer et al. 1987)
4.47 (CPC-RV correlation, Terada et al. 1987)
4.07 (OECD 81 method, Kerler & Schönherr 1988)
5.04 (HPLC-RT correlation, Shigeoka et al. 1988; quoted, Saito et al. 1993)
5.00 (batch equilibration-UV, Beltrame et al. 1988)
5.06 (calculated-CLOGP, Müller & Klein 1992)
5.01, 5.38 (quoted, calculated-original UNIFAC, Chen et al. 1993)
5.24 (EPA CLOGP Data Base, Hulzebos et al. 1993)
5.18 (recommended, LOGKOW databank, Sangster 1993)
5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
5.12 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

3.75 (fish, Statham et al. 1976)
3.04 (fish, Körte et al. 1978)
2.89 (fathead minnow, 32-d exposure, Veith et al. 1979)
2.89 (fathead minnow, calculated value, Veith et al. 1979b)
2.64 (algae, calculated, Geyer et al. 1981)
2.00 (trout, Hattula et al. 1981)
3.04, 3.10, 3.02 (activated sludge, algae, golden orfe, Freitag et al. 1982)
2.54 (mussel Mytilus edulis, quoted average, Geyer et al. 1982)
3.69 (calculated-K_{org}, Mackay 1982)
1.60 (killifish, Trujillo et al. 1982)
1.86, 1.72, 1.60 (low-PCP flowing, high-PCP flowing, high-PCP static soft water; Brockway et al. 1984)
1.66, 1.62, 1.26 (low-PCP flowing, high-PCP flowing, high-PCP static hard water; Brockway et al. 1984)
3.10 (alga chlorella fusca in culture flasks, Geyer et al. 1984)
3.10, 2.72 (algae: exptl, calculated-K_{org}, Geyer et al. 1984)
3.10, 3.02, 3.04 (algae, fish, sludge, Klein et al. 1984)
3.00 (quoted, LeBlanc 1984)
3.04, 3.10, 2.42 (activated sludge, algae, golden ide, Freitag et al. 1985)
0.57 (human fat, Geyer et al. 1987)
2.99 (zebrafish, Butte et al. 1987)
0.46 (15 °C, initial concn. 1.0 mg/L uptake by Allolobophora caliginosa at 24 hours, Haque & Ebing 1988)
0.38 (15 °C, initial concn. 10.0 mg/L uptake by Allolobophora caliginosa at 24 h, Haque & Ebing 1988)
0.80 (whole Allolobophora caliginosa/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
1.35 (whole Lumbricus terrestris/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
2.80, 2.63 (earthworm E. fetida andrei: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
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-2.66 (daily intake/cow adipose tissue, Travis & Arms 1988)
4.10 (rainbow trout, field bioaccumulation, Thomann 1989)
4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
2.97 (P. hoyi, Landrum & Dupuis 1990)
2.11 (M. relicta, Landrum & Dupuis 1990)
2.16–2.53 (soft tissue of freshwater mussel, Mäkelä & Oikari 1990)
2.33; 3.21 (flagfish: whole fish; fish lipid, Smith et al. 1990)
2.78, 2.11, 1.72 (goldfish at pH 7, pH 8, pH 9, Stehly & Hayton 1990)
2.89, 1.11 (fathead minnow, bluegill; Saito et al. 1992)
3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)

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

2.95 (soil, calculated-$K_{OW}$, Kenaga & Goring 1980)
3.11–5.65 (soil, calculated-$K_{OW}$ model of Karickhoff et al. 1979, Sabljic 1987a, b)
3.17–4.54 (soil, calculated-$K_{OW}$ model of Kenaga & Goring 1980, Sabljic 1987a, b)
3.37–3.69 (soil, calculated-$K_{OW}$ model of Briggs 1981, Sabljic 1987a, b)
3.00–5.54 (soil, calculated-$K_{OW}$ model of Means et al. 1982, Sabljic 1987a, b)
2.21–4.49 (soil, calculated-$K_{OW}$ model of Chiou et al. 1983, Sabljic 1987a, b)
4.52 (sediment, Schellenberg et al. 1984)
2.95, 3.41 (quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
3.73 (quoted average of Kenaga & Goring 1980 and Schellenberg et al. 1984 values, Sabljic 1987a, b)
3.46 (soil, calculated-MCI $\chi$, Sabljic 1987a, b)
2.95 (soil, calculated-MCI $\chi$, Bahnick & Doucette 1988)
4.04 (estimated, HPLC-$k'$ correlation, Hodson & Williams 1988)
4.40 (calculated, Lagas 1988)
3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
5.17, 3.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
5.58, 3.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)

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

Volatile/evaporation: $t_\frac{1}{2} = 84$ h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);

$k = 0.028$ d$^{-1}$ for nondissociated PCP, assuming diffusion coefficient in air to be $7 \times 10^{-4}$ m$^2$/s and in water $7 \times 10^{-10}$ m$^2$/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);

calculated rate constant $k = 5 \times 10^{-4}$ d$^{-1}$ to $1 \times 10^{-7}$ d$^{-1}$ for total PCP (Crossland & Wolff 1985).

Photolysis: calculated photolysis $t_\frac{1}{2} = 4.75$ h from observed rate $k = 3.4 \times 10^{-4}$ s$^{-1}$ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm$^2$ between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);

photolysis $t_\frac{1}{2} = 1.5$ d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);

photolytic $t_\frac{1}{2} = 10–15$ d (Brockway et al. 1984);

$k = 0.23$ to 0.46 d$^{-1}$ for direct photo-transformation, is the main loss process for PCP from ponds, with $t_\frac{1}{2} = 1.5$ to 3.0 d (Crossland & Wolff 1985);

photo-transformation rate constant $k = 0.6$ h$^{-1}$ with $t_\frac{1}{2} = 1$ h for distilled water in summer (mean temperature 25°C) and $k = 0.37$ h$^{-1}$ with $t_\frac{1}{2} = 2$ h in winter (mean temperature 11°C); $k = 0.37$ h$^{-1}$ with $t_\frac{1}{2} = 2$ h for both poisoned estuarine water and estuarine water in summer and $k = 0.27$ h$^{-1}$ with $t_\frac{1}{2} = 3$ h in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

photo-mineralization rate constant $k = 0.11$ h$^{-1}$ with $t_\frac{1}{2} = 6$ d for distilled water in summer (mean temperature 25°C) and $k = 0.049$ h$^{-1}$ with $t_\frac{1}{2} = 14$ d in winter (mean temperature 11°C); $k = 0.12$ h$^{-1}$ with $t_\frac{1}{2} = 6$ d
for poisoned estuarine water in summer and $k = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ in winter; $k = 0.25 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for estuarine water in summer and $0.10 \text{ h}^{-1}$ with half-life of 7 d for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

phototransformation $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Bjørndal 1988);

aqueous photolysis $t_{1/2} = 1–110 \text{ h}$ (Hwang et al. 1986; Sugiuira et al. 1984; selected, Howard et al. 1991);

$\text{photodegradation rate constant } k = 0.60 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 1.0 \text{ h} \text{ (summer), } k = 0.37 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 2 \text{ h} \text{ (winter) in distilled water; and } k = 0.37 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 2 \text{ h} \text{ (summer), } k = 0.27 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 3.0 \text{ h} \text{ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).}$

Oxidation: rate constant $k >> 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983);

photooxidation $t_{1/2} = 66–3480 \text{ h}$ in water, based on reported reaction rate constants for reaction of OH and RO$_2$ radicals with phenol class in aqueous solution (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

rate constant $k = (0.2 \pm 5.5) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ C$ (Tratnyek & Hoigné 1991);

atmospheric $t_{1/2} < 24 \text{ h}$ at noon in mid-summer to $t_{1/2} = 216 \text{ h}$ in January at latitude of 41.79°N for reaction with OH radicals (Bunce et al. 1991).

Hydrolysis: is not expected to occur (Crossland & Wolff 1985).

Biodegradation: $t_{1/2} = 1800–2160 \text{ h}$ and $480–\infty \text{ h}$ to obtain 75% degradation in mineral medium and seawater, respectively (De Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 552–4272 \text{ h}$, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 1008–36480 \text{ h}$, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aerobic degradation rate constant $k = 0.0017 \text{ L} \text{ µg}^{-1} \text{ d}^{-1}$ (Moos et al. 1983);

microbial degradation negligible in darkness (Hwang et al. 1986);

degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).

Biotransformation: degradation rate $k = 3 \times 10^{-14} \text{ mol-cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Half-Lives in the Environment:

Air: $t_{1/2} = 139.2–1392 \text{ h}$, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photolysis $t_{1/2} = 6.5 \text{ h}$ in noontime summer sunshine (Howard 1991);

$\text{photodegradation rate constant } k = 0.60 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 1.0 \text{ h} \text{ (summer), } k = 0.37 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 2 \text{ h} \text{ (winter) in distilled water; and } k = 0.37 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 2 \text{ h} \text{ (summer), } k = 0.27 \text{ h}^{-1} \text{ corresponding to } t_{1/2} = 3.0 \text{ h} \text{ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).}$

Surface water: calculated photolysis $t_{1/2} = 4.75 \text{ h}$ from a determined rate $k = 3.4 \times 10^{-4} \text{ s}^{-1}$ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm$^2$ between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);

photolysis $t_{1/2} = 1.5 \text{ d}$ was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

photolytic $t_{1/2} = 10–15 \text{ d}$ (Brockway et al. 1984);

rate constant $k >> 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);
\[ t_{1/2} = 1.5 \text{ to } 3.0 \text{ d for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);} \]
\[ t_{1/2} = 1 \text{ h in summer, } t_{1/2} = 2 \text{ h in winter for distilled water; } t_{1/2} = 2 \text{ h in summer, } t_{1/2} = 3 \text{ h in winter for estuarine water; } t_{1/2} = 2 \text{ h in summer, } t_{1/2} = 3 \text{ h in winter for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986);} \]
\[ t_{1/2} = 6 \text{ d in summer, } t_{1/2} = 14 \text{ d in winter for distilled water; } t_{1/2} = 3 \text{ d in summer, } t_{1/2} = 7 \text{ d in winter for estuarine water; } t_{1/2} = 6 \text{ d in summer, } t_{1/2} = 10 \text{ d in winter for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);} \]
\[ t_{1/2} = 0.75 \text{ h and } 0.96 \text{ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);} \]
\[ t_{1/2} = 1–110 \text{ h, based on aqueous photolysis half-life (Howard et al. 1991);} \]
\[ \text{photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991);} \]
\[ \text{photodegradation } t_{1/2} = 1.0 \text{ h in summer, } 2.0 \text{ h in winter in distilled water and } t_{1/2} = 2.0 \text{ h in summer, } 3.0 \text{ h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).} \]

Ground water: \[ t_{1/2} = 1104–36,480 \text{ h, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et al. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).} \]

Sediment:
Soil: disappearance \[ t_{1/2} = 23.2 \text{ d from Kooyenburg soil, } t_{1/2} = 47.9 \text{ d from Holten soil with earthworm } E. \text{ fetida andrei and } t_{1/2} = 27.4 \text{ d from Kooyenburg soil, } t_{1/2} = 31.8 \text{ d from Holten soil with earthworm } L. \text{ rubellus (van Gestel & Ma 1988);} \]
\[ t_{1/2} = 552–4272 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);} \]
\[ t_{1/2} = 12.0 \text{ d in an acidic clay soil with <1.0\% organic matter and } t_{1/2} = 6.7 \text{ d in a slightly basic sandy loam soil with 3.25\% organic matter, based on aerobic batch lab. microcosm experiments (Loehr & Matthews 1992).} \]

Biota: biological \[ t_{1/2} \sim 30 \text{ d in guppy } L. \text{ reticulatus (Landner et al. 1977);} \]
edition \[ t_{1/2} = 23, 9.3, 6.9, \text{ and } 6.2 \text{ h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);} \]
estimated \[ t_{1/2} = 7.0 \text{ d in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);} \]
clearance from flagfish: \[ t_{1/2} = 0.68 \text{ d from whole fish and } t_{1/2} = 0.68 \text{ d from fish lipid (Smith et al. 1990).} \]
18.1.1.67 Permethrin

Common Name: Permethrin
Synonym: Ambush, Dragnet, Ectiban, Exmin, FMC 33297, FMC 41665, ICI-PP 557, Kafil, Kestrel, NDRC-143, NIA 33297, Niagara 33297, Outflank, Outflank-stockade, Perthrine, Picket, Pounce, Pramex, S 3151, SBP-1513, Talcord, WL 43479

Chemical Name: 3-phenoxybenzyl (1RS, 3RS; 1RS, 3SR)-3(2,2-dichlorovinyl)-2,2-dimethylcyclo-propanecarboxylate; 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl ester

Uses: insecticide to control overwintering forms of spider mites, aphids, and scale insects on fruit trees, vines, olives, bananas and ornamentals; used as herbicides to control grass and broadleaf weeds in umbelliferous crops, and in tree nurseries; also used as acaricide and surfactant.

CAS Registry No: 52645-53-1
Molecular Formula: C_{21}H_{20}Cl_{2}O_{3}
Molecular Weight: 391.288

Melting Point (°C):
- liquid (tech. grade, Worthing & Hance 1991)
- 34 (Lide 2003)

Boiling Point (°C):
- 200 (at 0.01 mmHg, Hartley & Kidd 1987; Milne 1995)
- 200 (tech. grade at 0.1 mmHg, Worthing & Hance 1991; Tomlin 1994)
- 220 (at 0.05 mmHg, Montgomery 1993)
- >290 (Tomlin 1994)

Density (g/cm³ at 20°C):
- 1.19–1.27 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
- 1.214 (tech. grade at 25°C, Worthing & Hance 1991)

Molar Volume (cm³/mol):
- 431 (calculated-Le Bas method at normal boiling point)
- 318.1 (calculated-density)

Dissociation Constant, pKₐ:

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: 0.816 (mp at 34°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 0.20 (Martin & Worthing 1977)
- 0.04 (shake flask-GC, Coats & O’Donnell-Jefferey 1979)
- 0.2 (Spencer 1982)
- 0.05 (in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)
- 0.20 (20°C, Hartley & Kidd 1987; Tomlin 1994)
- 0.20 (30°C, Worthing & Walker 1987, 1991)
- 0.2 (20°C, Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 4.8 × 10⁻⁶ (cis isomer, Barlow 1978)
- 4.9 × 10⁻⁶ (cis isomer, Wells et al. 1986)
- 3.7 × 10⁻⁶ (trans isomer, Barlow 1978)
- 3.1 × 10⁻⁶ (trans isomer, Wells et al. 1986)
- 4.5 × 10⁻⁵ (Hartley & Kidd 1987; Tomlin 1994)
1.0 × 10⁻⁵ (cis isomer, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
8.1 × 10⁻⁶ (trans isomer, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
1.3 × 10⁻⁶ (tech. grade at 20°C, Worthing & Hance 1991)
2.5 × 10⁻⁶ (pure cis isomer at 20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.5 × 10⁻⁶ (pre trans isomer at 20°C, Worthing & Hance 1991; Tomlin 1994)
1.7 × 10⁻⁶ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.4 × 10⁻⁵ (cis isomer, Knudsen effusion, measured range 40–80°C, Goodman 1997)
8.71 × 10⁻⁶ (solid P, converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.0867 (wetted wall column-GC, Fendinger & Glotfelty 1990)
2.50 × 10⁻⁵ (calculated-bond contribution method, Meylan & Howard 1991)
0.00486 (20°C, calculated-P/C, Montgomery 1993)
0.0157 (20–25°C, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:
3.49 (shake flask-GC, Coats & O’Donnell-Jefferey 1979)
6.60 (calculated, Briggs 1981)
6.50 (shake flask-GC, Schimmel et al. 1983)
6.2 ± 0.9 (cis-form, HPLC-RT correlation, Muir et al. 1985)
5.7 ± 0.7 (trans-form, HPLC-RT correlation, Muir et al. 1985)
6.10 (tech. grade at 20°C, Worthing & Hance 1991; Tomlin 1994)
6.67 (HPLC-RT correlation, Hu & Leng 1992)
2.88–6.10 (Montgomery 1993)
6.50 (recommended, Sangster 1993)
6.10 (Milne 1995)
5.85 (RP-HPLC-RT correlation, Finizio et al. 1997)
5.73 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
3.18 (calculated-S, Kenaga 1980)
3.28 (Schimmel et al. 1983)
3.23, 3.49, 3.52 (Pimephales promelas, Spehar et al. 1983;)
1.49–1.84 (trans-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.08–2.13 (trans-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70 (trans-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
0.90–2.22 (cis-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.46–2.62 (cis-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.32–2.47 (cis-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
4.71, 4.83 (oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
4.71, 4.83 (sheepshead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.29, 3.39 (Oncorhynchus mykiss, Muir et al. 1994; quoted, Devillers et al. 1996)
2.79 (quoted, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
4.03 (calculated-S, Kenaga 1980)
2.76 (cis-form, silt, K_P on 34% DOC, Muir et al. 1985)
2.64 (cis-form, clay, K_P on 77% DOC, Muir et al. 1985)
2.64 (trans-form, silt, K_P on 23% DOC, Muir et al. 1985)
2.64 (trans-form, clay, K_P on 0% DOC, Muir et al. 1985)
5.25 (soil, calculated-χ and fragment contribution, Meylan et al. 1992)
5.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
1.32–2.79 (Montgomery 1993)
4.80 (soil, calculated-MCI χ, Sabljic et al. 1995)
4.42, 4.35 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: photodegradation rate constant $k = 1.73 \times 10^{-3} \, \text{min}^{-1}$ and $t_{1/2} = 400 \, \text{min}$ with TiO$_2$ as catalyst after 20 h irradiation at 222 nm (Hidaka et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

$\frac{dC}{dt} = kC$ with $k =$ $1.24 \times 10^{-2} \, \text{h}^{-1}$ for bacteria strain $A. \ sobria$ with $t_{1/2} = 56 \, \text{h}$, $k =$ $1.13 \times 10^{-2} \, \text{h}^{-1}$ for $E. \ carotovora$ with $t_{1/2} = 61 \, \text{h}$, $k =$ $8.66 \times 10^{-3} \, \text{h}^{-1}$ for $Y. \ frederiksenii$ with $t_{1/2} = 80 \, \text{h}$ and $k =$ $1.43 \times 10^{-3} \, \text{h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 485 \, \text{d}$ in aqueous soil-free phase ($cis$-permethrin, Lee et al. 2004)

$\frac{dC}{dt} = 1.50 \times 10^{-2} \, \text{h}^{-1}$ for $A. \ sobria$ with $t_{1/2} = 45 \, \text{h}$, $k =$ $1.51 \times 10^{-2} \, \text{h}^{-1}$ for $E. \ carotovora$ with $t_{1/2} = 46 \, \text{h}$, $k =$ $1.85 \times 10^{-2} \, \text{h}^{-1}$ for $Y. \ frederiksenii$ with $t_{1/2} = 37 \, \text{h}$ and $k =$ $2.85 \times 10^{-3} \, \text{h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 259 \, \text{d}$ in aqueous soil-free phase ($trans$-permethrin, Lee et al. 2004)

Biotransformation:

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

$k_1$ = $1.5–2.3 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in pond sediment-water system for $trans$-permethrin, 96-h exposure, Muir et al. 1983)

$k_1$ = $1.50 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in river sediment-water system for $trans$-permethrin, 96-h exposure, Muir et al. 1983)

$k_1$ = $3.3–12.1 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in sediment (sand)-water system for $trans$-permethrin, 96-h exposure, Muir et al. 1983)

$k_1$ = $4.9–14.7 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in sediment (sand)-water system for $trans$-permethrin, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2$ = $0.041 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in pond sediment-water system for $trans$-permethrin, calculated by concentration decay curve, Muir et al. 1983)

$k_2$ = $0.021 \, \text{h}^{-1}$ ($Chironomus \ tentans$ larvae in sediment (sand)-water system for $trans$-permethrin, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air:
Surface water: $t_{1/2} > 21 \, \text{d}$ in 100 mL pesticide-seawater solution under indoor conditions, $t_{1/2} = 14 \, \text{d}$ under outdoor light conditions and $t_{1/2} > 14 \, \text{d}$ under outdoor dark conditions (Schimmel et al. 1983);
biodegradation half-lives by bacteria strains: $t_{1/2} = 56 \, \text{h}$ by $A. \ sobria$, $t_{1/2} = 61 \, \text{h}$ by $E. \ carotovora$, $t_{1/2} = 80 \, \text{h}$ by $Y. \ frederiksenii$ and $t_{1/2} = 485 \, \text{d}$ for the control, uninoculated solution for $cis$-permethrin; $t_{1/2} = 45 \, \text{h}$ by $A. \ sobria$, $t_{1/2} = 46 \, \text{h}$ by $E. \ carotovora$, $t_{1/2} = 37 \, \text{h}$ by $Y. \ frederiksenii$ and $t_{1/2} = 259 \, \text{d}$ for the control, uninoculated solution for $trans$-permethrin (Lee et al. 2004)

Ground water:

Sediment: half-lives in 10 grams sediment/100 mL pesticide-seawater solution: $t_{1/2} < 2.5 \, \text{d}$ for untreated sediment and $t_{1/2} > 28 \, \text{d}$ for sterile sediment (Schimmel et al. 1983).

Soil: reported $t_{1/2} < 38 \, \text{d}$ in soil containing 1.3–51.3% organic matter at pH 4.2–7.7 (Holmstead et al. 1978; quoted, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994); selected field $t_{1/2} = 30 \, \text{d}$ (Wauchope et al. 1992; Hornsby et al. 1996); soil $t_{1/2} = 30 \, \text{d}$ (Pait et al. 1992);
$\text{soil } t_{1/2} = 32 \, \text{d}$ for forest soil (Dowd et al. 1993).

Biota: elimination $t_{1/2} \approx 16.7 \, \text{h}$ in pond sediment-water, $t_{1/2} = 32.9 \, \text{h}$ in sand-water systems ($Chironomus \ tentans$ larvae, Muir et al. 1983)
TABLE 18.1.1.67.1
Reported vapor pressures of cis-permethrin at various temperatures

Goodman 1997

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>1.4 × 10⁻³</td>
</tr>
<tr>
<td>50</td>
<td>1.10 × 10⁻⁴</td>
</tr>
<tr>
<td>60</td>
<td>5.30 × 10⁻⁴</td>
</tr>
<tr>
<td>70</td>
<td>2.30 × 10⁻³</td>
</tr>
<tr>
<td>80</td>
<td>8.90 × 10⁻³</td>
</tr>
</tbody>
</table>

log P = A – B/(T/K)

A 18.70
B 7677

FIGURE 18.1.1.67.1 Logarithm of vapor pressure versus reciprocal temperature for cis-permethrin.
18.1.1.68 Phenthoate

Common Name: Phenthoate
Synonym: Cidial, Elsan
Chemical Name: ethyl 2-dimethoxyphosphinothioylthio(phenyl)acetate; ethyl 2-dimethoxy-thiophosphorylthio-2-phenylacetate; S-α-ethoxycarbonylbenzyl O,O-dimethyl phosphorodithioate; ethyl α-[(dimethoxy-phosphinothioyl)thio]benzeneacetate
Uses: insecticide to control aphids, scale insects, jassids, lepidopterous larvae, bollworms, mealybugs, psyllids, thrips, spider mites, etc. in citrus fruit, pome fruit, olives, cotton, cereals, rice, coffee, tea, sunflower, sugar cane, tobacco, ornamentals, and vegetables; also used as acaricide and for control of mosquito larvae.

CAS Registry No: 2597-03-7
Molecular Formula: C12H17O4PS2
Molecular Weight: 320.364
Melting Point (°C):
17.5 (Khan 1980; Spencer 1982)
17–18 (Worthing & Hance 1991; Tomlin 1994)
Boiling Point (°C): 78–80 (Spencer 1982)
Density (g/cm³ at 20°C):
1.226 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Molar Volume (cm³/mol):
261.3 (calculated from density)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ∆H_fus (kJ/mol):
Entropy of Fusion, ∆S_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 K/ml K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
200 (Martin & Worthing 1977)
11 (20°C, Khan 1980; Hartley & Kidd 1987)
Vapor Pressure (Pa at 25°C or as indicated):
0.005 (40°C, Hartley & Kidd 1987)
0.0053 (40°C, Worthing & Hance 1991; Tomlin 1994)
3.5 × 10⁻⁴ (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
9.77 × 10⁻⁴; 2.45 × 10⁻⁴, 6.76 × 10⁻⁴ (gradient GC method; estimation using modified Watson method: Sugden’s paracho, McGowan’s paracho, Tsuzuki 2000)
Henry’s Law Constant (Pa·m³/mol):
0.01019 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow}:
2.89 (shake flask-GC, Kanazawa 1981)
3.96 (shake flask/slow stirring-GC, De Bruijn et al. 1991)
3.69 (Worthing & Hance 1991; Tomlin 1994)
3.32 (RP-HPLC-RT correlation, Saito et al. 1993)
3.69 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.49 (calculated-S, Kenaga 1980)
1.56 (topmouth gudgeon *Pseudorasbora parva*, Kanazawa 1981)
2.85 (whole body willow shiner after 168 h exposure, Tsuda et al. 1992)
1.57, 1.43, 1.30, 1.51 (whole body carp: 24 h, 72 h, 120 h and 168 h; Tsuda et al. 1993)

Sorption Partition Coefficient, log $K_{OC}$:
2.38 (soil, calculated-S, Kenaga 1980)

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

**Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**
- excretion rate constant $k = 0.05$ h$^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
- excretion rate constant $k = 0.52$ h$^{-1}$ with $t_\frac{1}{2} = 1.3$ h (Tsuda et al. 1993).

**Half-Lives in the Environment:**

**Air:**

**Surface water:**

**Ground water:**

**Sediment:**
- Soil: selected field $t_\frac{1}{2} = 11$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
- $t_\frac{1}{2} = 10$ d in silty clay loam and other soils (Tomlin 1994).

**Biota:**
- excretion rate constant $k = 0.05$ h$^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
- excretion rate constant $k = 0.52$ h$^{-1}$ with $t_\frac{1}{2} = 1.3$ h (Tsuda et al. 1993).
18.1.1.69 Phorate

Common Name: Phorate
Synonym: AC 3911, American Cyanamid 3911, ENT 24042, Foraat, Gramitox, Granutox, Rampart, Thimate, Thimet, Timet, Vegfu, Vergfru foratox

Chemical Name: \( O,O-\text{diethyl-S-(ethylthio)methyl phosphorodithioate} \); \( O,O-\text{diethyl-S-ethylmercaptomethyl dithiophosphate} \); phosphorodithioic acid \( O,O-\text{diethyl S-(ethylthio)methyl} \) ester

Uses: insecticide to control mites, chewing and sucking insects in fruits and vegetables, cotton, and some ornamentals; also used as acaricide and nematicide.

CAS Registry No: 298-02-2

Molecular Formula: \( C_7H_{17}O_2PS_3 \)
Molecular Weight: 260.378

Melting Point (°C):
-42.9 (Spencer 1982)
<−15 (Montgomery 1993; Lide 2003)

Boiling Point (°C):
118–120 (at 0.8 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
125–127 (at 2 mmHg, Budavari 1989; Milne 1995)
118–120 (tech. grade at 0.8 mmHg, Worthing & Hance 1991)

Density (g/cm³ at 20°C):
1.156 (25°C, Merck Index 1989; Montgomery 1993; Milne 1995)
1.167 (tech. grade at 25°C, Spencer 1982; Worthing & Hance 1991)

Molar Volume (cm³/mol):
259.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, \( pK_a \):

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 \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), \( F: 1.0 \)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
19 (26°C, 95% pure, shake flask-GC, Lord & Burt 1964)
14 (15°C, shake flask-GC, Lord & Burt 1964)
85 (Günther et al. 1968)
70 (Melnikov 1971; Briggs 1981)
50 (Spencer 1973, 1982)
50 (Martin & Worthing 1977; Hartley & Kidd 1987)
80–85 (Wauchope 1978)
20 (shake flask-GC, Felsot & Dahm 1979)
17.9 (20°C, shake flask-GC, Bowman & Sans 1979, 1983b)
50 (room temp., Worthing & Walker 1987; Budavari 1989, Milne 1995)
50 (tech. grade at room temp., Worthing & Hance 1991)
20 (24°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
0.112 (20°C, Wolfdietrich 1965; Spencer 1973, 1982)
0.25 (Woolford 1975)
0.148 (gas saturation method, Sutherland et al. 1980)
0.074 (gas saturation-GC, Kim et al. 1984)
0.042 (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.769</td>
<td>calculated-P/C, Jury et al. 1984, 1987a, 1990; Jury &amp; Ghodrati 1989</td>
</tr>
<tr>
<td>0.65</td>
<td>(20°C, calculated-P/C, Suntio et al. 1988)</td>
</tr>
<tr>
<td>0.648</td>
<td>(20–24°C, calculated-P/C, Montgomery 1993)</td>
</tr>
<tr>
<td>1.010</td>
<td>(calculated-P/C, this work)</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>3.33</td>
<td>shake flask-GC</td>
<td>Felsot &amp; Dahm 1979</td>
</tr>
<tr>
<td>2.92</td>
<td>(shake flask-UV, Lord et al. 1980)</td>
<td></td>
</tr>
<tr>
<td>4.26</td>
<td>shake flask-GC</td>
<td>Briggs 1981</td>
</tr>
<tr>
<td>4.26</td>
<td>(22°C, shake flask-GC, Bowman &amp; Sans 1983b)</td>
<td></td>
</tr>
<tr>
<td>3.24</td>
<td>(shake flask, Log P Database, Hansch &amp; Leo 1987)</td>
<td></td>
</tr>
<tr>
<td>3.92</td>
<td>(Worthing &amp; Hance 1991)</td>
<td></td>
</tr>
<tr>
<td>2.91–3.92</td>
<td>(Montgomery 1993)</td>
<td></td>
</tr>
<tr>
<td>2.92</td>
<td>(recommended, Sangster 1993)</td>
<td></td>
</tr>
<tr>
<td>3.92</td>
<td>(Milne 1995)</td>
<td></td>
</tr>
<tr>
<td>3.56</td>
<td>(selected, Hansch et al. 1995)</td>
<td></td>
</tr>
<tr>
<td>4.25</td>
<td>(RP-HPLC-RT correlation, Finizio et al. 1997)</td>
<td></td>
</tr>
<tr>
<td>3.94</td>
<td>(RP-HPLC-RT correlation using short ODP column, Donovan &amp; Pescatore 2002)</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>1.83</td>
<td>(calculated-S, calculated-$K_{OC}$, Kenaga 1980)</td>
<td></td>
</tr>
<tr>
<td>2.34</td>
<td>(earthworms, Lord et al. 1980)</td>
<td></td>
</tr>
<tr>
<td>−1.70</td>
<td>(vegetation, correlated-$K_{OW}$, Travis &amp; Arms 1988)</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Method</th>
<th>Source</th>
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<tbody>
<tr>
<td>3.51</td>
<td>(soil, Hamaker &amp; Thompson 1972; Kenaga 1980; Kenaga &amp; Goring 1980)</td>
<td></td>
</tr>
<tr>
<td>2.71</td>
<td>(soil, calculated-S as per Kenaga &amp; Goring 1978, Kenaga 1980)</td>
<td></td>
</tr>
<tr>
<td>2.82</td>
<td>(soil, sorption isotherm, converted form reported log $K_{OM}$ of 2.82, Briggs 1981)</td>
<td></td>
</tr>
<tr>
<td>2.32–3.60</td>
<td>(reported as log $K_{OM}$, Mingelgrin &amp; Gerstl 1983)</td>
<td></td>
</tr>
<tr>
<td>2.82</td>
<td>(screening model calculations, Jury et al. 1987a, b; Jury &amp; Ghodrati 1989)</td>
<td></td>
</tr>
<tr>
<td>2.58, 2.88</td>
<td>(reported as log $K_{OM}$, estimated as log $K_{OM}$, Magee 1991)</td>
<td></td>
</tr>
<tr>
<td>2.73</td>
<td>(soil, Worthing &amp; Hance 1991)</td>
<td></td>
</tr>
<tr>
<td>2.64</td>
<td>(estimated-QSAR &amp; SPARC, Kollig 1993)</td>
<td></td>
</tr>
<tr>
<td>2.51–2.80</td>
<td>(Montgomery 1993)</td>
<td></td>
</tr>
<tr>
<td>2.82</td>
<td>(selected, Lohninger 1994)</td>
<td></td>
</tr>
<tr>
<td>2.70</td>
<td>(soil, calculated-MCI $^{1}$, Sabljc et al. 1995)</td>
<td></td>
</tr>
<tr>
<td>2.70, 2.98, 3.12</td>
<td>(soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)</td>
<td></td>
</tr>
<tr>
<td>2.63</td>
<td>(soil: organic carbon OC -0.5%, average, Delle Site 2001)</td>
<td></td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:

Volatileization:

Photolysis:

Oxidation:
Insecticides 3961

Hydrolysis: neutral hydrolysis rate constant \( k = 7.2 \times 10^{-3} \text{ h}^{-1} \) with a calculated \( t_{1/2} = 96 \text{ h} \) at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993);
calculated rate constant \( k = 100 \times 10^{-12} \text{ cm}^3/\text{molecule} \cdot \text{s} \) for the vapor-phase reaction with hydroxyl radical in air (Winer & Atkinson 1990);
\( t_{1/2} = 3.2 \text{ d} \) at pH 7 and \( t_{1/2} = 3.9 \text{ d} \) at pH 9 (Worthing & Hance 1991);
rate constant \( k = 62 \text{ yr}^{-1} \) at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: \( t_{1/2} = 82 \text{ d} \) for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983);
\( t_{1/2} = 82 \text{ d} \) in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghorati 1989);
first-order rate constant \( k = -0.0403 \text{ h}^{-1} \) in nonsterile sediment and \( k = -0.0209 \text{ h}^{-1} \) in sterile sediment by shake-tests at Range Point and first-order rate constant \( k = -0.0206 \text{ h}^{-1} \) in nonsterile water and \( k = -0.0186 \text{ h}^{-1} \) in sterile water by shake-tests at Range Point (Walker et al. 1988);
first-order rate constants \( k = -0.0241 \text{ h}^{-1} \) in nonsterile sediment and \( k = -0.0185 \text{ h}^{-1} \) in sterile sediment by shake-tests at Davis Bayou and first-order rate constants \( k = -0.0262 \text{ h}^{-1} \) in nonsterile water and \( k = -0.0185 \text{ h}^{-1} \) in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil: \( t_{1/2} = 68 \text{ d} \) in a sandy soil (Way & Scopes 1968; quoted, Montgomery 1993);
estimated persistence of 2 wk (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
persistence of less than one month (Wauchope 1978);
biodegradation \( t_{1/2} = 82 \text{ d} \) in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);
\( t_{1/2} = 2–14 \text{ d} \) (Worthing & Hance 1991);
estimated field \( t_{1/2} = 60 \text{ d} \) (Wauchope et al. 1992; quoted, Richards & Baker 1993; selected, Halfon et al. 1996; Hornsby et al. 1996);
soil \( t_{1/2} = 25 \text{ d} \) (Pait et al. 1992).
Biota: \( t_{1/2} = 1.4 \text{ d} \) half-lives in coastal Bermuda grass and alfalfa (Leuck & Bowman 1970; quoted, Montgomery 1993) and \( t_{1/2} = 3.6 \text{ d} \) (Dobson et al. 1960; quoted, Montgomery 1993);
biochemical \( t_{1/2} = 82 \text{ d} \) from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).
**18.1.1.70 Phosmet**

![Chemical Structure of Phosmet](image)

Common Name: Phosmet  
Synonym: APPA, Decemthion, Decemthion p-6, EN1 25,705, Ftalophos, Imidan, Percolate, Phthalophos, Prolate, R 1504, Safidon, Smidan, Stauffer R-1504  
Chemical Name: O,O-dimethyl S-phthalimidomethyl phosphorodithioate; N-dimethoxyphosphino-thioyiethylo-thiophthalimide; S-[(1,3-dihydro-1,3-dioxo-2H-isooindol-2-yl)methyl] O,O-dimethyl phosphorodithioate; phosphoro-dithioic acid, S-[(1,3-dihydro-1,3-dioxo-2H-isooindol-2-yl)methyl] O,O-dimethyl ester  

**Uses:** nonsystemic acaricide and insecticide.  
**CAS Registry No:** 732-11-6  
**Molecular Formula:** C₁₁H₁₂NO₄PS₂  
**Molecular Weight:** 317.321  
**Melting Point (°C):**  
72.0–72.7, 66.5–69.5 (pure, technical grade, Montgomery 1993; Tomlin 1994)  
72 (Lide 2003)  
**Boiling Point (°C):**  
decompose rapidly >100°C (Montgomery 1993)  
**Density (g/cm³ at 20°C):**  
**Molar Volume (cm³/mol):**  
263.3 (calculated-Le Bas method at normal boiling point)  
**Dissociation Constant, pKₐ:**  
**Enthalpy of Fusion, ΔH₅₀ (kJ/mol):**  
30.96 (Plato & Glasgow 1969)  
**Entropy of Fusion, ΔS₅₀ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS₅₀ = 56 J/mol K), F:** 0.346 (mp at 72°C)  
0.3 (20°C, Suntio et al. 1988)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
25 (Bright et al. 1950, Melnikov 1971; Spencer 1982)  
25 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)  
22–25 (Montgomery 1993)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
6.03 × 10⁻⁴ (20°C, Freed et al. 1977)  
0.133 (50°C, Spencer 1982; Hartley & Kidd 1987)  
6.03 × 10⁻⁵, 0.133 (30, 50°C, Montgomery 1993)  
6.50 × 10⁻⁵ (Tomlin 1994)  
2.0 × 10⁻⁵, 5.90 × 10⁻⁵ (gradient GC method; quoted lit. value, Tsuzuki 2000)  
**Henry’s Law Constant (Pa·m³/mol):**  
9.50 × 10⁻⁴ (calculated-P/C, Suntio et al. 1988)  
9.53 × 10⁻⁴ (calculated-P/C, Montgomery 1993)  
7.62 × 10⁻⁴ (calculated-P/C, this work)  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
2.83 (20°C, shake flask-GC, Chiou et al. 1977)  
2.83 (Rao & Davidson 1980)
Insecticides

2.78 (22°C, shake flask-GC, Bowman & Sans 1983)
2.81 (shake flask/slow stirring-GC, De Bruijn & Hermens 1991)
2.78–3.04 (Montgomery 1993)
2.78 (recommended, Sangster 1993)
2.95 (Tomlin 1994)
3.40 (Milne 1995)
2.78 (recommended, Hansch et al. 1995)
3.06 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
0.90 (bluegill sunfish/fathead minnows, Saito et al. 1992)
1.04 (channel catfish, Saito et al. 1992)
1.56 (av. whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
0.23 (av. whole body carp after 24–168 h exposure, Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC}:
2.91 (soil, Wauchope et al. 1992, Hornsby et al. 1996)
2.06, 2.34 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:
Photolysis: t_{1/2} = 53.25 h for absorbance wavelength at 243 nm (Montgomery 1993).
Oxidation:
Hydrolysis: t_{1/2} = 7.2 d at pH 6.1 and t_{1/2} = 7.1 h at pH 7.4 at 20°C; t_{1/2} = 1.1 h at 37.5°C (Freed et al. 1979; quoted, Montgomery 1993);
\hspace{1cm} t_{1/2} = 13 d at pH 4.5, t_{1/2} < 12 h at pH 7 and t_{1/2} < 4 h at pH 8.3 in buffered aqueous solution at 20°C (Montgomery 1993);
\hspace{1cm} t_{1/2} = 7.0 d at pH 6.1, and t_{1/2} = 7.1 h at pH 7.4 at 20°C (Lartiges & Garrigues 1995).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
\hspace{1cm} k_2 = 0.28 h^{-1} (whole body willow shiner, Tsuda et al. 1992)

Half-Lives in the Environment:

Air:
Surface water: t_{1/2} = 33 d at 6°C, t_{1/2} = 5 d at 22°C in darkness for Milli-Q water at pH 6.1 (Lartiges & Garrigues 1995).
Ground water:

Sediment:
Soil: field t_{1/2} = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota: t_{1/2} = 6.5 d in Bermuda grass (Montgomery 1993).
Common Name: Pirimicarb  
Synonym: Pirimor, AphiX, Abol, Aficida, Fernos, Rapid  
Chemical Name: 2-dimethylamino-5,6-dimethylpyrimidin-4-yl dimethylcarbamate  
CAS Registry No: 23103-98-2  
Uses: insecticide  
Molecular Formula: C₁₁H₁₈N₄O₂  
Molecular Weight: 238.287  
Melting Point (°C):  
90.5 (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994; Lide 2003)  
Boiling Point (°C):  
Density (g/cm³ at 20°C):  
1.21 (Tomlin 1994)  
Molar Volume (cm³/mol):  
Dissociation Constant, pKₐ:  
Enthalpy of Fusion, ΔHₘₐ₃ (kJ/mol):  
Entropy of Fusion, ΔSₘₐ₃ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₘ₃ = 56 J/mol K), F: 0.228 (mp at 90.5°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
2700 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)  
2000 (pH 4, 20°C, Tomlin 1994)  
2700 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
Vapor Pressure (Pa at 25°C):  
0.00097 (Tomlin 1994)  
0.004 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log Kₐₐw:  
1.70 (Tomlin 1994)  
1.70 (recommended, Hansch et al. 1995)  
1.70 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)  
Octanol/Air Partition Coefficient, log Kₐₐ:  
Bioconcentration Factor, log BCF or log Kₐ:  
0.845 (calculated-Solubility, Kenaga 1980b)  
Sorption Partition Coefficient, log Kₐₐ:  
1.76 (soil, Kenaga 1980b)  
1.57 (soil, estimated and selected value, Augustijn-Beckers et al. 1994)  
1.36 (soil, estimated and selected, Hornsby et al. 1996)  
1.90, 1.52 (soil: quoted, calculated-MCI χ, Meylan et al. 1992)
Insecticides

1.90 (soil, calculated-MCI \( \chi \), Sabljic et al 1995)
1.90; 2.30, 1.80 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis: aqueous solutions are unstable to UV light with \( t_{\frac{1}{2}} < 1 \) d at pH 5.7 or 9 (Tomlin 1994).

Oxidation:

Hydrolysis:

Biodegradation: \( t_{\frac{1}{2}} = 7–234 \) d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aqueous solutions are unstable to UV light with \( t_{\frac{1}{2}} < 1 \) d at pH 5.7 or 9 (Tomlin 1994).

Ground water:

Sediment:

Soil: \( t_{\frac{1}{2}} = 7–234 \) d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994);

field \( t_{\frac{1}{2}} \sim 10 \) d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:
18.1.1.72 Propoxur

Common Name: Propoxur
Synonym: Baygon, Blattanex, Under, arprocarb, PHC, Sendran, Suncide, Aracarb, Tugon Fliegendugel
Chemical Name: 2-(1-methylethoxy)phenol methyl carbamate
CAS Registry No: 114-26-1
Uses: insecticide to control cockroaches, flies, fleas, mosquitoes, bugs, ants, millipedes and other insect pests in food storage areas, houses, animal houses, etc.; also to control sucking and chewing insects in fruits, vegetables, ornamentals, vines, maize, lucerne, soya beans, cotton, sugar cane, rice cocoa, forestry, etc.
Molecular Formula: C₁₁H₁₅NO₃
Molecular Weight: 209.242
Melting Point (°C)
91.50 (Spencer 1982; Howard 1991; Kühne et al. 1995)
84–87 (Montgomery 1993)
87 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
244.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔH₉₈ (kJ/mol):
Entropy of Fusion, ΔS₉₈ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉₈ = 56 J/mol K), F: 0.246 (mp at 87°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
2000 (Kenaga 1980; Kanazawa 1981)
1860 (20°C, shake flask-GC, Bowman & Sans 1983)
Vapor Pressure (Pa at 25°C or as indicated):
1.333 (120°C, Melnikov 1971; Spencer 1973, 1982)
4.13 × 10⁻⁴ (20°C, Hartley & Graham-Bryce 1980)
4.13 × 10⁻³ (20°C, selected exptl. value from literature, Kim 1985)
0.0593, 0.0113 (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
4.00 × 10⁻⁴ (20°C, Howard 1991)
1.30 × 10⁻³ (20°C, Montgomery 1993; Siebers et al. 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.1308 (20°C, calculated-P/C, Suntio et al. 1988)
4.46 × 10⁻⁵ (calculated-P/C, Howard 1991)
1.32 × 10⁻⁴ (calculated-P/C, Montgomery 1993)
1.40 × 10⁻⁴ (calculated-P/C, Siebers et al. 1994)
1.98 × 10⁻⁶ (calculated-P/C, this work)
### Octanol/Water Partition Coefficient, log $K_{OW}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.52</td>
<td>(shake flask-UV, Fujita et al. 1974)</td>
</tr>
<tr>
<td>1.50</td>
<td>(Hansch &amp; Leo 1979)</td>
</tr>
<tr>
<td>1.45</td>
<td>(Rao &amp; Davidson 1980)</td>
</tr>
<tr>
<td>1.52</td>
<td>(Kenaga &amp; Goring 1980; Kanazawa 1981)</td>
</tr>
<tr>
<td>1.552</td>
<td>(shake flask-GC, Bowman &amp; Sans 1983)</td>
</tr>
<tr>
<td>1.52</td>
<td>(Hansch &amp; Leo 1985)</td>
</tr>
<tr>
<td>1.75</td>
<td>(RP-HPLC-RT correlation, Trapp &amp; Pussemier 1991)</td>
</tr>
<tr>
<td>1.45–1.56</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>1.52</td>
<td>(recommended, Sangster 1993)</td>
</tr>
<tr>
<td>1.52</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>1.99</td>
<td>(RP-HPLC-RT correlation, Nakamura et al. 2001)</td>
</tr>
</tbody>
</table>

### Bioconcentration Factor, log $BCF$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.924</td>
<td>(calculated, Howard 1991)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.67</td>
<td>(measurements for average of 2 soils, Kanazawa 1981, 1989)</td>
</tr>
<tr>
<td>1.86</td>
<td>(calculated, Howard 1991)</td>
</tr>
<tr>
<td>1.48</td>
<td>(soil, Wauchope et al. 1992; Hornsby et al. 1996)</td>
</tr>
<tr>
<td>0.48–1.97</td>
<td>(Montgomery 1993)</td>
</tr>
<tr>
<td>1.48</td>
<td>(estimated-chemical structure, Lohninger 1994)</td>
</tr>
<tr>
<td>1.67</td>
<td>(soil, calculated-MCI $\chi$, Sabljic et al. 1995)</td>
</tr>
<tr>
<td>1.63, 1.88</td>
<td>(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)</td>
</tr>
</tbody>
</table>

### Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

#### Volatilization:

- Photolysis: atmospheric and/or aqueous photolysis $t_{1/2} = 62.5–87.9$ h, based on measured rate of photolysis on bean leaves in sunlight (Ivie & Casida 1971; quoted, Howard et al. 1991) and in aqueous solution under simulated sunlight (Jensen-Korte et al. 1987; quoted, Howard et al. 1991);
- Photolyze in water with $t_{1/2} = 88$ h and decreased with humic material to 13–41 h; $t_{1/2} = 87.9$ h in water when irradiated with light >290 nm (Howard 1991).

#### Oxidation:

- Photooxidation $t_{1/2} = 0.71–7.1$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- Vapor-phase photooxidation $t_{1/2} = 4.3$ h for reaction with ambient OH radical (Howard 1991).

#### Hydrolysis:

- $t_{1/2} = 40$ min at pH 10 and 20°C, hydrolyzes at a rate of 1.5% d$^{-1}$ in 1% aqueous solution at pH 7 (Spencer 1982);
- $t_{1/2} = 16, 1.6$ and 0.17 d at pH 8, 9, 10, but stable between pH 3–7; $t_{1/2} = 40$ min at pH 10 (Howard 1991);
- $t_{1/2} = 290$ d at pH 7, $t_{1/2} = 17.9$ d at pH 8 and $t_{1/2} = 48$ min at pH 10 (Montgomery et al. 1993);
- Hydrolysis $t_{1/2} = 16$ d, 1.6 d and 4.2 h in water at pH 8, 9 and 10 (Aly & El-Dib 1971; quoted, Montgomery 1993).

#### Biodegradation:

- Aquatic aerobic $t_{1/2} = 168–672$ h, based on unacclimated aquatic aerobic screening test data (Gummer 1979; Kanazawa 1987; quoted, Howard et al. 1991); aquatic anaerobic $t_{1/2} = 672–2688$ h, based on estimated unacclimated aerobic anaerobic biodegradation half-life (Howard et al. 1991);
- $t_{1/2} = 44$ d under aerobic conditions and $t_{1/2} = 59$ d under anaerobic conditions in water used a combination of activated sludge, silt loam soil and sediment as an inoculum; $t_{1/2} = 78$ d under aerobic conditions and $t_{1/2} = 125$ d under anaerobic conditions at pH 6.9 (Howard 1991).

#### Biotransformation:

- Metabolism rate $k = 3.70 \times 10^{-3}$ h$^{-1}$ leading to an irradiated moist soil $t_{1/2} = 180$ h (Graebing & Chib 2004)

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

### Half-Lives in the Environment:

- Air: $t_{1/2} = 0.71–7.1$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $t_{1/2} \sim 4$ h reacting with photochemically produced hydroxyl radical in air (Howard 1991).
Surface water: \( t_{1/2} = 38–672 \) h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
\( t_{1/2} = 1 \) d to 1 wk by degradation, photolyze rapidly with \( t_{1/2} = 13 \) to 88 h (Howard 1991).

Ground water: \( t_{1/2} = 38–1344 \) h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} = 38–672 \) h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Field \( t_{1/2} = 14–50 \) d (Wauchope et al. 1992)

On sandy loam soil: first-order rate constants for photolytic decline, \( k = 1.65 \times 10^{-3} \) h\(^{-1}\) irradiated in moisture-maintained soil, \( k = 0.91 \times 10^{-3} \) h\(^{-1}\) irradiated in air-dried soil, \( k = 0.91 \times 10^{-3} \) h\(^{-1}\) in dark control moist soil and \( k = 0.23 \times 10^{-3} \) h\(^{-1}\) in dark control air-dried sandy loam soil from Madia, CA. The initial metabolism rate \( k = 3.70 \times 10^{-3} \) h\(^{-1}\) leading to an irradiated moist soil \( t_{1/2} = 180 \) h; in the dark \( t_{1/2} = 380 \) h in moist soil Graebing & Chib 2004)

Biota:
18.1.1.73 Ronnel

Common Name: Ronnel
Chemical Name: O,O-dimethyl O-(2,4,5-trichlorophenyl)thiophosphate; O,O-dimethyl O-2,4,5-trichlorophenyl phosphorothioate; phosphoric acid O,O-dimethyl O-(2,4,5-trichlorophenyl)ester
Uses: insecticide.
CAS Registry No: 299-84-3
Molecular Formula: C₈H₈Cl₃O₃PS
Molecular Weight: 321.546
Melting Point (°C):
40–42 (Spencer 1982)
41 (Montgomery 1993; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.48 (25°C, Montgomery 1993)
Molar Volume (cm³/mol):
257.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔHₘᵤₛ (kJ/mol):
23.85 (Plato & Glasgow 1969)
Entergy of Fusion, ΔSₘᵤₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘᵤₛ = 56 J/mol K), F: 0.697 (mp at 41°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
44 (Günther et al. 1968; Melnikov 1971)
1.08 (20°C, shake flask-GC, Chio et al. 1977)
1.08 (20–25°C, shake flask-GC/ECD, Freed et al. 1979)
2.5 (20°C, Spencer 1982)
0.60 (20°C, shake flask-GC, Bowman & Sans 1979, 1983)
0.98 (20°C, corrected supercooled liq. value, shake flask-GC, Bowman & Sans 1979, 83)
6.0 (Dow Chemical unpublished data, Kenaga 1980a, b; Kenaga & Goring 1980)
40 (22°C, Khan 1980)
1.0 (20°C, shake flask-HPLC, Ellgehausen et al. 1981)
1.61 (20°C, selected, Suntio et al. 1988)
40 (Montgomery 1993; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
0.0533 (20°C, Eichler 1965; Melnikov 1971)
0.0071 (20–25°C, Freed et al. 1979)
1.067 (Spencer 1982)
0.0017 (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
0.0011 (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
0.016 (20°C, selected, Suntio et al. 1988)
0.0045 (20°C, Montgomery 1993)
Henry’s Law Constant (Pa-m³/mol at 25°C or as indicated):
3.22 (20°C, calculated-P/C, Suntio et al. 1988)
0.857 (20–25°C, calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log $K_{ow}$ at 25°C or as indicated:
- 4.88  
  (20°C, shake flask-GC, Chiou et al. 1977)
- 4.67  
  (Kenaga 1980b; Kenaga & Goring 1980)
- 4.88  
  (20–25°C, shake flask-GC/ECD, Freed et al. 1979)
- 5.34  
  (shake flask-HPLC, Ellgehausen et al. 1981)
- 4.81  
  (20°C, shake flask-GC, Bowman & Sans 1983)
- 5.068 ± 0.004  
  (shake flask/slow-stirring method, De Bruijn et al. 1989)
- 4.67–5.068  
  (Montgomery 1993)
- 4.88  
  (recommended, Sangster 1993)
- 5.07  
  (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log $BCF$:
- 2.35  
  (calculated-S, Kenaga 1980a, b)
- −1.38  
  (average beef fat diet, Kenaga 1980b)
- 4.64  
  (guppy *Poecilia reticulata*, lipid wt basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log $K_{oc}$:
- 3.20  
  (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
- 2.90  
  (soil, calculated-MCI $\chi$, Gerstl & Helling 1987)
- 2.76  
  (calculated, Montgomery 1993)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: estimated $t_{1/2} \sim 3$ d at pH 6 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_1 = 0.01337$ mL g$^{-1}$ d$^{-1}$ (guppy, 0.5–420 h exposure, De Bruijn & Hermens 1991)
- $k_2 = 0.38$ d$^{-1}$ (guppy, De Bruijn & Hermens 1991)
- $k_2 = 0.14$ d$^{-1}$ (calculated-$K_{ow}$, De Bruijn & Hermens 1991)

Half-Lives in the Environment:
18.1.1.74 Terbufos

Common Name: Terbufos
Synonym: AC 92100, Counter, ST-100
Chemical Name: \( S-\text{(tert-butylthio)methyl} O,O-\text{diethyl phosphorodithioate} \)
\( S-[(1,1\text{-dimethylethyl} \text{thio})\text{methyl}] O,O-\text{diethyl phosphorodithioate} \)
\( \text{phosphorodithioic acid} S-\text{(tert-butylthio)methyl} O,O-\text{diethyl ester} \)

Uses: insecticide in soil to control insects and also used as nematocide to control nematodes in beet, maize, cotton, sorghum, onions, cabbage, and bananas.

CAS Registry No: 13071-79-9
Molecular Formula: \( \text{C}_9\text{H}_{21}\text{O}_2\text{PS}_3 \)
Molecular Weight: 288.431

Melting Point (°C):

Boiling Point (°C):
69 (at 0.01 mmHg, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
312 (Brecken-Folse et al. 1994; Howe et al. 1994)

Density (g/cm\(^3\) at 20°C):

Molar Volume (cm\(^3\)/mol):
261 (24°C, calculated from density)

Dissociation Constant, pK\(_a\):

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/m\(^3\) or mg/L at 25°C or as indicated):
- 12 (Martin & Worthing 1977)
- 5.07 (shake flask-GC, Felsot & Dahm 1979)
- \( \leq 10 \) (Spencer 1982)
- 5.5 (19°C, shake flask-GC, Bowman & Sans 1983a, b)
- 10–15 (Worthing & Hance 1991)
- 15 (calculated, Pait et al. 1992)
- 0.10 (Howe et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated):
- 0.0346 (Worthing & Hance 1991; Tomlin 1994)
- 0.0427 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.0351 (20°C, Montgomery 1993)
- 0.0174; 0.0346 (liquid \( P_t \), GC-RT correlation; quoted lit., Donovan 1996)
- 0.0148; 0.00912, 0.0151 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)

Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
- 2.463 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
- 3.68 (shake flask-LSC, Felsot & Dahm 1979)
- 2.22 (Rao & Davidson 1980)
Bioconcentration Factor, log BCF:

- 2.73 (topmouth gudgeon, Metcalf & Sanborn 1975)
- 2.18 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
- 1.0 \((Triaenodes\ tardus,\ Belluck\ &\ Felsot\ 1981)\)

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

- 3.04 (soil, calculated-S per Kenaga & Goring 1978, Kenaga 1980)
- 2.76, 3.29 (quoted, calculated-MCI \(\chi\), Gerstl & Helling 1987)
- 2.46–3.03 (Montgomery 1993)
- 2.82 (soil, calculated-MCI \(\chi\), Sabljic et al. 1995)
- 2.80, 3.30 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

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

Half-Lives in the Environment:

- Soil: \(t_{1/2} = 9–27\) d in soil (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
- selected field \(t_{1/2} = 5.0\) d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996);
- soil \(t_{1/2} = 5\) d (Pait et al. 1992).
18.1.1.75 Thiodicarb

Common Name: Thiodicarb
Synonym: Bismethomyl thioether, Dicarbosulf
Chemical Name: dimethyl N,N′-(thiobis(methylimino)carbonyloxy)bis(ethanimidothioate)
CAS Registry No: 59669-26-0
Uses: insecticide/molluscicide
Molecular Formula: C_{10}H_{18}N_{4}O_{4}S_{3}
Molecular Weight: 354.470

Melting Point (°C):
- 168–172 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
- 173 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C): 1.40 (Montgomery 1993)

Molar Volume (cm³/mol):

Dissociation Constant, pKₐ:

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: 0.0353 (mp at 173°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 35 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Vapor Pressure (Pa at 25°C):
- 0.0043 (20°C, Hartley & Kidd 1987; Montgomery 1993)
- 0.0054 (20°C, Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol):
- 0.044 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{ow}:
- 1.70 (shake flask-HPLC, Drabel & Bachmann 1983)
- 1.2–1.6 (Montgomery 1993)
- 1.70 (recommended, Sangster 1993)
- 1.70 (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_{ow}:
- 1.81–3.07; 2.54 (quoted range of reported data; mean, Wauchope et al. 1992)
- 2.54 (soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.06; 2.25; 2.10–2.69; 2.32–2.52; 2.57 (various soils: clay; loam; sand; sandy loam; silty loam (quoted, Montgomery 1993))
1.81–3.07 (various soils, Montgomery 1993)
2.54; 1.68, 2.57 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Hydrolysis: $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);
stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: hydrolysis $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);
stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).
Ground water:
Sediment:
Soil: $t_{1/2} = 3–8$ d in various soils (Hartley & Kidd 1987)
field $t_{1/2} = 7$ d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:
18.1.1.76 Toxaphene

Common Name: Toxaphene
Chemical Name: mixtures of chlorinated camphene and bornane
Uses: pesticide used primarily on lettuce, cotton, corn, tomatoes, peanuts, wheat and soybean.
CAS Registry No: 8001-35-2
Molecular Formula: C\textsubscript{10}H\textsubscript{16}Cl\textsubscript{8}
Molecular Weight: 413.812

Note: A large number of isomers exist, thus the commercial product is a mixture and the properties below should be regarded as average values for the specific mixture. Considerable variability in properties is thus expected.

Melting Point (°C):
- 65–90 (Howard 1991; Montgomery 1993; Milne 1995)
- 35 (dec., Milne 1995)

Boiling Point (°C):
- 246, 351, 360 (estimated from structure, Tucker et al. 1983)

Density (g/cm\textsuperscript{3} at 20°C):
- 1.65 (25°C, Spencer 1982; Montgomery 1993)

Molar Volume (cm\textsuperscript{3}/mol):
- 358.8 (calculated-Le Bas method at normal boiling point)
- 366.8 (calculated-Le Bas method)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

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

Fugacity Ratio at 20°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$:
- 0.30 (Mackay et al. 1986)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and the reported temperature dependence equations):
- 3.0 (Brooks 1974)
- 0.74 (generator column-GC/ECD, Weil et al. 1974)
- 0.40 (Leonard et al. 1976; Wauchope 1978)
- 0.40 (Sanborn et al. 1976; Weber et al. 1980)
- 0.40 (Martin & Worthing 1977)
- 0.50 (shake flask-GC, Paris et al. 1977)
- 3.0 (22°C, Khan 1980; Spencer 1982)
- 0.3–3.0 (U.S. EPA 1984; McLean et al 1988)
- 3.0 (20°C, selected, Suntio et al. 1988)
- 0.55 (20°C, Montgomery 1993)
- 0.63 (calculated from vapor pressure and HLC, Wania & Mackay 1993)

\[
\log [C/(mol/m^3)] = 0.77 - \frac{1071}{(T/K)} \quad (\text{Wania & Mackay 1993})
\]
- 3.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- $4.0 \times 10^{-5}$ (20°C, Spencer 1973)
- 27–53 (Brooks 1974; Khan 1980)
- $1.3 \times 10^{-4}$ (Leonard et al. 1976)
- $1.3 \times 10^{-4}$ (20–25°C, Weber et al. 1980)
- $1.3 \times 10^{-4}$ (30°C, Seiber et al. 1981)
- $2.0 \times 10^{-5}$, $4.5 \times 10^{-5}$, 0.667 (estimated-bp, Tucker et al. 1983)
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):  

- 27.0 (U.S. EPA 1984; quoted, McLean et al. 1988)  
- 8.92 \times 10^{-4} (20°C, estimated, Murphy et al. 1987)  
- 0.0005 (20°C, selected, Suntio et al. 1988)  
- 27–54 (20°C, Montgomery 1993)  
- 0.0016 (calculated from the eq. below, Wania & Mackay 1993)  

\[ \log \left( \frac{P}{Pa} \right) = 12.25 - \frac{4487}{(T/K)} \]  

- 5.3 \times 10^{-4} (20–25°C, selected, Hornsby et al. 1996)  

(2.3–7.10) \times 10^{-4} (supercooled P_L, capillary GC-RT correlation, for 21 toxaphene components-chlorinatedbornane and camphene congeners, Bidleman et al. 2003)  

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

- 3.52 (shake flask-GC, Paris et al. 1977)  
- 5.30 (HPLC-RT correlation, Veith et al. 1979)  
- 3.23 (Rao & Davidson 1980)  
- 5.28 (Veith & Kosian 1983)  
- 4.83 (from Veith’s personal communication, Zaroogian et al. 1985)  
- 5.50 (Garten & Trabalka 1983)  
- 3.85 (Ryan et al. 1988)  
- 4.63 (estimated-QSAR & SPARC, Kollig 1993)  
- 3.23–5.50 (Montgomery 1993)  
- 4.77–6.64 (range for 36 toxaphene components/congeners, shake flask/slow stirring-GC/ECD, Fisk et al. 1999)  

Bioconcentration Factor, log BCF: 

- -2.79 (beef biotransfer factor log B_b, correlated-K_{OW}, Radeleff et al. 1952; Claborn et al. 1953,60)  
- -3.20 (milk biotransfer factor log B_m, correlated-K_{OW}, Saha 1969)  
- 3.53 (Bacillus subtilis, Paris et al. 1975, 1977)  
- 3.72 (Flavobacterium harrisonii, Paris et al. 1975, 1977)  
- 4.23 (Aspergillus sp., Paris et al. 1975, 1977)  
- 4.04 (Chlorella prenoidosa, Paris et al. 1975, 1977)  
- 3.63 (Gambusia, Sanborn et al. 1976)  
- 4.84 (fathead minnows, Mayer et al. 1977)  
- 3.51–4.23 (microorganisms, Paris et al. 1977)  
- 3.59 (pinfish, 4-d exposure, Schimmel et al. 1977; Veith & Kosian 1983)  
- 3.64 (sheepshead minnow, 4-d exposure, Schimmel et al. 1977)
Insecticides

3.49–4.52, 2.60–3.08 (fish, shrimp, Reish et al. 1978)
4.42, 3.63 (fish: flowing water, static water; Kenaga & Goring 1980)
4.42, 3.02 (fish, calculated-solubility, Kenaga 1980)
3.59 (pinfish, Veith & Kosian 1983)
3.64 (sheepshead minnow, Veith & Kosian 1983)
3.81, 3.72 (fish: flowing system, microcosm, Garten & Trabalka 1983)
3.84, 3.98 (algae: snail, Garten & Trabalka 1983)
3.44, 3.41 (oyster, calculated-$K_{ow}$ and models, Zaroogian et al. 1985)
3.44, 3.41 (pinfish, calculated-$K_{ow}$ and models, Zaroogian et al. 1985)
3.44, 3.41 (sheepshead minnow, calculated-$K_{ow}$ & models, Zaroogian et al. 1985)
4.52, 6.44 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.57, 6.50 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.84, 6.06 (fathead minnow, flow-through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.80, 5.80 (fathead minnow, flow-through 150-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
>4.73, >5.84 (channel catfish, flow-through 100-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.04, 3.204 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

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

3.86 (calculated-S, Kenaga 1980; quoted, Howard 1991)
4.32 (soil, screening model calculations, Jury et al. 1987a, b, 1990; Jury & Ghodrati 1989)
5.32 (sediment, Bomberger et al. 1983; quoted, Howard 1991)
3.17 (calculated-$K_{ow}$ as per Kenaga & Goring 1980, Chapman 1989)
4.31 (estimated-QSAR and SPARC, Kollig 1993)
3.18 (calculated, Montgomery 1993)
5.00 (20–25°C, selected, Hornsby et al. 1996)

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

Volatilization: volatilization $t_{1/2} = 2650$ d from chemical below soil surface (Jury et al. 1990).

Photolysis:

Hydrolysis: estimated $t_{1/2} > 10$ yr at pH 5–8 and 25°C (Callahan et al. 1979; quoted, Howard 1991)

$$k = (8.0 \pm 2.2) \times 10^{-5} \text{ h}^{-1} \text{ at pH 7 with a calculated } t_{1/2} = 10 \text{ yr (Ellington et al. 1987, 1988)}$$

$$k = 7.0 \times 10^{-2} \text{ yr}^{-1} \text{ at pH 7.0 and 25°C (Kollig 1993)}. $$

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:

$$t_{1/2} = 4–5 \text{ d for the vapor-phase reaction with hydroxyl radicals (Howard 1991)}$$

$$k(aq.) = 8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)}$$

$$k(aq.) < 1.3 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 5.6 and 21°C, with } t_{1/2} > 7 \text{ h at pH 7 (Yao & Haag 1991)}.$$  

$$k(aq.) = (1.2–8.1) \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at 24 ± 1°C (Haag & Yao 1992)}$$

Biodegradation: very resistant to degradation in soils with reported from $t_{1/2} = 0.8$ yr (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991).

Biotransformation:

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

$$k_1 = 0.016 \text{ d}^{-1} \text{ with } t_{1/2} = 43 \text{ d and } k_2 = 0.022 \text{ d}^{-1} \text{ with } t_{1/2} = 32 \text{ d for food concn of 21 ng/g and 136 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C}_7\text{-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)}$$

$$k_1 = 0.007 \text{ d}^{-1} \text{ with } t_{1/2} = 95 \text{ d and } k_2 = 0.016 \text{ d}^{-1} \text{ with } t_{1/2} = 43 \text{ d for food concn of 18 ng/g and 121 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C}_8\text{-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)}$$
k_2 = 0.008 d^{-1} with t_{1/2} = 83 d and k_2 = 0.017 d^{-1} with t_{1/2} = 42 d for food concn of 17 ng/g and 134 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for C_{9-CHB} toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)
k_2 = 0.068 yr^{-1}, 0.093 yr^{-1}, 0.160 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (lipid-adjusted, Glassmeyer et al. 2000)
k_2 = 0.085 yr^{-1}, 0.086 yr^{-1}, 0.165 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (wet weight, Glassmeyer et al. 2000)

Half-Lives in the Environment:
Air: t_{1/2} = 4–5 d for the vapor-phase reaction with hydroxyl radicals (GEMS 1986; quoted, Howard 1991).
Surface water: measured k < 1.3 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with t_{1/2} > 7 h at pH 7 (Yao & Haag 1991);
half-lives in lake water: t_{1/2} = 18–31 yr in Lake Superior, t_{1/2} = 5–8 yr in Lake Michigan, t_{1/2} ~ 8.5 yr in Lake Huron and t_{1/2} ~ 6 yr in Lake Ontario (Glassmeyer et al. 2000).

Ground water:
Sediment:
Soil: very persistent with reported half-life from t_{1/2} = 0.8 yr (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991);
t_{1/2} > 50 d when subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988)
measured dissipation rate k = 0.010 d^{-1} (Seiber et al. 1979; quoted, Nash 1988);
t_{1/2} = 9 d in screening model calculations (Jury et al. 1987b);
estimated dissipation rate k = 0.0011 and 0.013 d^{-1} (Nash 1988);
t_{1/2} = 3650 d for volatilization to atmosphere from chemical below soil surface (Jury et al. 1990);
field t_{1/2} = 9 d (20–25°C, selected, Hornsby et al. 1996)
t_{1/2} = 0.8–14 yr in soil, t_{1/2} = 10–18 yr in the environment (Geyer et al. 2000)
Biota: field t_{1/2} = 15.6 d in fruit tree leaves (Decker et al. 1950; quoted, Nash 1983);
microagroecosystem t_{1/2} = 19 d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
field t_{1/2} ca. 6.3 d in cotton canopy (Willis et al. 1980; quoted, Nash 1983);
t_{1/2} = 524 d for white suckers, and t_{1/2} = 232 to 322 d for lake trout (total toxaphene, Delorme et al. 1993);
average fish half-lives in the Great Lakes. t_{1/2} = 9.1 yr in Lake Michigan, t_{1/2} = 7.7 yr in Lake Huron and t_{1/2} = 4.3 yr in Lake Ontario (lake trout, Glassmeyer et al. 2000)
Depuration t_{1/2} = 32–96 d for a 30-d uptake and 160-d depuration studies (Juvenile rainbow trout, Fisk et al. 1998)

### Table 18.1.1.76.1
Reported Henry’s law constants of toxaphene at various temperatures

<table>
<thead>
<tr>
<th>Jantunen et al. 2000</th>
</tr>
</thead>
<tbody>
<tr>
<td>air stripping-GC</td>
</tr>
<tr>
<td>( t/°C )</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>35</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>( \log H = A - B/(T/K) )</td>
</tr>
<tr>
<td>A</td>
</tr>
<tr>
<td>B</td>
</tr>
</tbody>
</table>

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FIGURE 18.1.1.76.1 Logarithm of Henry's law constant versus reciprocal temperature for toxaphene.
Common Name: Trichlorfon

Synonym: Aerol 1, Agroforotox, Anthon, Bay 15922, Bayer 15922, Bilarcil, Bovinox, Britton, Britton, Cekufon, Chlorak, Chlorfos, Chlorphos, Chlorofotalm, Chloroxyphos, Ciclosom, Combat, Combat, Danex, DEP, Depthon, DETF, Dimetox, Dipterax, Diptevur, Ditrifon, Dylox, Dyrex, Dyvon, ENT 19763, Equino-acid, Flibol E, Forotox, Foschlor, Hypodermacid, Leivasom, Loisol, Masoten, Mazoten, Methyl chlorophos, Metifonate, Metrifonate, Metrphonate, NA 2783, NCI-C54831, Neguvon, Phoschlor, Proxol, Ricifon, Ritsifon, Soldep, Sotipox, Trichlorphon, Trichlorphene, Trinex, Tugon, Volfartol, Votexit, Wotexit

Chemical Name: dimethyl 2,2,2-trichloro-hydroxyethylphosphorate; 2,2,2-trichloro-hydroxy-ethylphosphoric acid dimethyl ester

Uses: insecticide to control flies and roaches.

CAS Registry No: 52-68-6

Molecular Formula: C₄H₈Cl₃O₄P

Molecular Weight: 257.437

Melting Point (°C): 77 (Lide 2003)

Boiling Point (°C): 100 (at 0.1 mmHg, Spencer 1973; Montgomery 1993; Milne 1995)

Density (g/cm³ at 20°C): 1.73 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol): 194.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pHₐ:

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: 0.309 (mp at 77°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

150000 (Dow Chemical data, Kenaga & Goring 1980)

Vapor Pressure (Pa at 25°C or as indicated):

0.00104 (20°C, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):

1.7 × 10⁻⁶ (20°C, calculated-P/C, Suntio et al. 1988)

1.7 × 10⁻⁶ (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log Kₐw:

0.48 (Dow Chemical data, Kenaga & Goring 1980)

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Insecticides

0.431 (shake flask-GC, Bowman & Sans 1983b)
0.76 (HPLC-RT correlation, Kawamoto & Urano 1989)
0.43–0.76 (Montgomery 1993)
0.51, 0.72 (shake flask, RP-HPLC-RT correlation, Siebaldi & Finizio 1993)
1.70 (22°C, shake flask, Brecken-Folse et al. 1994)
0.304 (12°C in reconstituted test water at pH 7.5, Howe et al. 1994)
0.51 (recommended, Sangster 1993)
0.43 (Tomlin 1994)
0.51 (recommended, Hansch et al. 1995)
0.72 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
–0.155 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log KOC:
0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.90 (correlated, Kawamoto & Urano 1989)
1.73 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
0.99–1.58 (Montgomery 1993)
1.90 (soil, calculated-MCI 1χ, Sabljic et al. 1995)
1.30 (sediment, estimated, Paraiba et al. 1999)
1.90; 1.87; 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: photooxidation t½ = 1–101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: first-order hydrolysis t½ = 68 h, based on first-order rate constant at pH 7 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);
t½ = 510 d at 22°C and at pH 4, t½ = 46 h at pH 7, and t½ < 30 min at pH 9 (Tomlin 1994).
Biodegradation: k(aerobic) = 0.28 d⁻¹ with t½ = 2.5 d at 20°C by aerobic activated sludge cultivated by an artificial sewage (batch contacting method, Kawamoto & Urano 1990)
aqueous aerobic t½ = 24–1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);
aqueous anaerobic t½ = 96–4320 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:
Half-Lives in the Environment:
Air: photooxidation t½ = 1–101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
reaction rate k = 1.90 × 10⁻⁴ min⁻¹ in air (Paraiba et al. 1999).
Surface water: t½ = 22–588 h, based on aqueous hydrolysis half-lives at pH 6 and 8 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);
t½ = 2.5 d at 20°C by aerobic activated sludge (Kawamoto & Urano 1990)
reaction rate k = 1.90 × 10⁻⁴ min⁻¹ in water (Paraiba et al. 1999).
Sediment: reaction rate k = 1.90 × 10⁻⁴ min⁻¹ in sediment (Paraiba et al. 1999).
Soil: t½ = 24–1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);
selected field t½ = 10 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996).
Biota:
# 18.2 SUMMARY TABLES

## TABLE 18.2.1
Common names, chemical names and physical properties of insecticides

<table>
<thead>
<tr>
<th>Name</th>
<th>Synonym</th>
<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>M.p. °C</th>
<th>Fugacity ratio, F at 25°C</th>
<th>pKₐ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acephate [30560-19-1]</td>
<td>Orthene</td>
<td>( O,S\text{-dimethyl acetylphosphoramo}dithioate )</td>
<td>( \text{C}<em>{10}\text{H}</em>{18}\text{NO}_{3}\text{PS} )</td>
<td>183.166</td>
<td>88</td>
<td>0.241</td>
<td></td>
</tr>
<tr>
<td>Aldicarb [116-06-3]</td>
<td>Temik</td>
<td>2-methyl-2-(methylthio)-propanaldehyde ( O\text{-}(\text{methylcarbamoyl}) \text{oxime} )</td>
<td>( \text{C}<em>{12}\text{H}</em>{17}\text{NO}_{3} )</td>
<td>190.263</td>
<td>99</td>
<td>0.188</td>
<td></td>
</tr>
<tr>
<td>Aldrin [309-00-2]</td>
<td>Aldrec, Aldrex, Aldrite, Octalene</td>
<td>1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endooxido-5,8-dimethano-naphthalene</td>
<td>( \text{C}<em>{12}\text{H}</em>{8}\text{Cl}_{6} )</td>
<td>364.910</td>
<td>104</td>
<td>0.168</td>
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<tr>
<td>Aminocarb [2032-59-9]</td>
<td>Matacil</td>
<td>4-dimethylamino-( \text{m} )-tolyl methylcarbamate</td>
<td>( \text{C}<em>{11}\text{H}</em>{16}\text{N}<em>{2}\text{O}</em>{2} )</td>
<td>208.257</td>
<td>94</td>
<td>0.210</td>
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<td>Azinphos-methyl [86-50-0]</td>
<td>Guthion</td>
<td>( O,O\text{-dimethyl-}[4\text{-oxo}-1,2,3\text{-benzotriazin-3(4H)-yl}methyl]\text{phosphorodithioate} )</td>
<td>( \text{C}<em>{10}\text{H}</em>{12}\text{N}<em>{3}\text{O}</em>{3}\text{PS}_{2} )</td>
<td>317.324</td>
<td>73</td>
<td>0.338</td>
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<tr>
<td>Bendiocarb [22781-23-3]</td>
<td>Bencarbate, Dycarb, Garvox, Multamat</td>
<td>2,2-dimethyl-1,3-benzodioxol-4-yl-methylcarbamate</td>
<td>( \text{C}<em>{11}\text{H}</em>{15}\text{NO}_{3} )</td>
<td>223.226</td>
<td>130</td>
<td>0.0933</td>
<td>8.8</td>
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<td>Bromophos [2104-96-3]</td>
<td>Nexion, S-1942, Omexan, Brofene</td>
<td>( O-4\text{-bromo-2,5-dichlorphenyl}-O,O\text{-dimethyl phosphorothioate} )</td>
<td>( \text{C}<em>{12}\text{H}</em>{11}\text{BrCl}_{2}\text{PS} )</td>
<td>317.999</td>
<td>54</td>
<td>0.519</td>
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<tr>
<td>Bromophos-ethyl [4824-78-6]</td>
<td>Nexagen, Filarol</td>
<td>( O\text{-}(4\text{-bromo-2,5-dichlorphenyl}) O,O\text{-diethyl phosphorothioate} )</td>
<td>( \text{C}<em>{10}\text{H}</em>{12}\text{O}<em>{3}\text{PS}</em>{2} )</td>
<td>394.049</td>
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<td>Carbaryl [63-25-2]</td>
<td>Sevin</td>
<td>1-naphthyl-N-methyl carbamate</td>
<td>( \text{C}<em>{11}\text{H}</em>{11}\text{NO}_{2} )</td>
<td>201.221</td>
<td>145</td>
<td>0.0665</td>
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<tr>
<td>Carbofuran [1563-66-2]</td>
<td>Furadan, Yaltax</td>
<td>2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate</td>
<td>( \text{C}<em>{12}\text{H}</em>{15}\text{NO}_{3} )</td>
<td>221.252</td>
<td>151</td>
<td>0.0580</td>
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<td>Carbofuran [1563-66-2]</td>
<td>Furadan, Yaltax</td>
<td>2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate</td>
<td>( \text{C}<em>{12}\text{H}</em>{15}\text{NO}_{3} )</td>
<td>221.252</td>
<td>151</td>
<td>0.0580</td>
<td></td>
</tr>
<tr>
<td>Carbofuran [786-19-6]</td>
<td>Furadan, Yaltax</td>
<td>S-chlorophenylthio methyl ( O,O\text{-diethyl phosphorothioate} )</td>
<td>( \text{C}<em>{11}\text{H}</em>{16}\text{Cl}<em>{2}\text{O}</em>{3}\text{PS} )</td>
<td>342.866</td>
<td>liquid</td>
<td>1</td>
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<tr>
<td>Carbosulfan [55285-14-8]</td>
<td>Marshal, Advantage Posse, FMC 35001</td>
<td>2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate</td>
<td>( \text{C}<em>{20}\text{H}</em>{32}\text{N}<em>{2}\text{O}</em>{3}\text{S} )</td>
<td>380.544</td>
<td>liquid</td>
<td>1</td>
<td></td>
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<td>Chlordane [57-74-9]</td>
<td>Aspon-chlordane, Chlorindan, Octchlor</td>
<td>1,2,4,5,7,8,8-octachloro-3( \alpha ),4,7,7( \alpha )-tetrahydro-4,7-methanoindane</td>
<td>( \text{C}<em>{10}\text{H}</em>{8}\text{Cl}_{8} )</td>
<td>409.779</td>
<td>106</td>
<td>0.160</td>
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<td>cis- or ( \alpha )-chlordane [5103-71-9]</td>
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<td>( \text{C}<em>{10}\text{H}</em>{6}\text{Cl}_{8} )</td>
<td>409.799</td>
<td>107–109</td>
<td>0.153</td>
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<tr>
<td>trans- or ( \beta )-chlordane [5103-74-2]</td>
<td></td>
<td></td>
<td>( \text{C}<em>{10}\text{H}</em>{6}\text{Cl}_{8} )</td>
<td>409.799</td>
<td>103–105</td>
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<td>( \gamma )-chlordane [5564-34-7]</td>
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<td>( \text{C}<em>{10}\text{H}</em>{6}\text{Cl}_{8} )</td>
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<td>technical grade[12789-03-6]</td>
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<td>Chlorfenvinphos [470-90-6]</td>
<td>Birlane, Sapecron</td>
<td>2-chloro-1-(2,4-dichlorophenyl) vinyl diethyl phosphate</td>
<td>( \text{C}<em>{12}\text{H}</em>{18}\text{Cl}<em>{2}\text{O}</em>{2}\text{PS} )</td>
<td>359.569</td>
<td>B19</td>
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<td>Chlorpyrifos [2921-88-2]</td>
<td>Brodan, Dursban, Dowco 179</td>
<td>( O,O\text{-diethyl } O,3,5,6\text{-trichloro } 2\text{-pyridyl phosphorothioate} )</td>
<td>( \text{C}<em>{12}\text{H}</em>{14}\text{Cl}<em>{2}\text{NO}</em>{3}\text{PS} )</td>
<td>350.586</td>
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<td>Chlorpyrifos-methyl [5598-13-0]</td>
<td>Reldan, Dowco 214</td>
<td>( O,O\text{-dimethyl } O,3,5,6\text{-trichloro } 2\text{-pyridyl phosphorothioate} )</td>
<td>( \text{C}<em>{12}\text{H}</em>{14}\text{Cl}<em>{2}\text{NO}</em>{3}\text{PS} )</td>
<td>322.534</td>
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<td>(RS)-α-cyano-3-phenoxybenzyl(Z)-(1RS,3RS)- (2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate</td>
<td>C$<em>{23}$H$</em>{19}$ClF$_3$NO$_3$</td>
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<td>o,p'-DDD [53-10-0]</td>
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<td>p,p'-DDE [72-55-9]</td>
<td>C$<em>{14}$H$</em>{10}$Cl$_4$</td>
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<td>o,p'-DDE [3424-82-6]</td>
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<td>p,p'-DDT [50-29-3]</td>
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<td>o,p'-DDT [789-02-6]</td>
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<td>Deltamethrin [62918-63-5]</td>
<td>C$<em>{22}$H$</em>{19}$Br$_2$NO$_3$</td>
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<td>Dicapthon [2463-84-5]</td>
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<td>Dialifor [10311-84-9]</td>
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<td>Demeton [8065-48-3]</td>
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<td>Demeton-S-methyl [919-86-8]</td>
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<td>Dichlorvos [62-73-7]</td>
<td>Vapona, Nuvan, DDVP,</td>
<td>2,2-dichlorovinyl-(O)-(O)-dimethyl phosphate</td>
<td>C₇H₅Cl₂O₄P</td>
<td>220.976</td>
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<td>Dicrotophos [141-66-2]</td>
<td>Carbicron, Ektafos,</td>
<td>((E))-2-dimethylcarbamoyl-1-methylvinyl dimethyl</td>
<td>C₈H₁₆NO₅P</td>
<td>237.191</td>
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<td>Dieldrin [60-57-1]</td>
<td>HEOD</td>
<td>1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4-endom-5,8-dimethanophthalene</td>
<td>C₁₂H₁₆Cl₈O</td>
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<td>Diflubenzuron</td>
<td>Deflubenzon, Dimilin</td>
<td>1-(4-chlorophenyl)-3-(2,6-difluoro-benzol) urea</td>
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<td>Dimethoate [60-51-5]</td>
<td>Cygon</td>
<td>(O)-(O)-dimethyl-(S)-(N)-methyl-carbamoyl-(S)-methyl phosphorodithioate</td>
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<td>Dinoseb [88-85-7]</td>
<td>Antox, Aretin, BNP 30,DNB P</td>
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<td>Di-Syston, Dithiosystox</td>
<td>(O)-(O)-diethyl-(S)-(S)-methylene bis(phosphorodithioate)</td>
<td>C₁₀H₂₂O₄P₂S₄</td>
<td>384.476</td>
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<td>Endosulfan [115-29-7]</td>
<td>Thiodan, Cyclodan,</td>
<td>5-norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfite</td>
<td>C₉H₆Cl₆O₃S</td>
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<td>α-Endosulfan</td>
<td>endrine, nendrin</td>
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<td>(\alpha)-ethylthio-(O)-tolyl methylcarbamate</td>
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<td>225.307</td>
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<td>Nialate, diethion</td>
<td>(O,(O),(O)-(O),(O)-tetraethyl-(S,(S)-methylene bis(phosphorodithioate)</td>
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<td>Fenitrothion [122-14-5]</td>
<td>Sumithion, Folithion</td>
<td>(O)-(O)-dimethyl-(O)-4-nitro-(m)-tolyl phosphorothioate</td>
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<td>Fenoxycarb [79127-80-3]</td>
<td>Logic, Pictyl, Varodo</td>
<td>ethyl 2-(4-phenoxyphenoxo)ethyl-carbamate</td>
<td>C₁₁H₁₉NO₄</td>
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<td>Fenpropathrin [64257–84–7]</td>
<td>Rodly, Danitol, Meothrin, S-3206</td>
<td>(R,(S)-o-cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropane carboxylate</td>
<td>C₂₂H₂₃NO₃</td>
<td>349.423</td>
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<td>Dassnit, Terracur</td>
<td>(O)-(O)-diethyl (O)-4-methylsulphonylphenyl phosphorothioate</td>
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<td>Fenthion [55-38-9]</td>
<td>Baytex, Baycid, Mercaptophos</td>
<td>$C_{10}H_{15}O_3PS_2$</td>
<td>278.328</td>
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<td>Fenvalerate [51630-58-1]</td>
<td>Sumicidin, Belmark, Pydrin</td>
<td>(RS)-α-cyano-3-phenoxbenzyl (RS)-2-(4-chlorophenyl)-3-methylbutyrate</td>
<td>$C_{25}H_{22}ClNO_2$</td>
<td>419.901</td>
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<td>Flucythrin [70124-77-5]</td>
<td>Cybolt, Cythrin, Pay-Off</td>
<td>(RS)-α-cyano-3-phenoxbenzyl (S)-(2-(4-difluoromethoxyphenyl)-3-methylbutyrate</td>
<td>$C_{26}H_{23}F_2NO_4$</td>
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<td>Dyfonate, Fonophos</td>
<td>O-ethyl-S-(phenyl $(RS)$-α-cyano-3-phenoxybenzyl $(RS)$-2-(4-chlorophenyl)-3-methylbutyrate</td>
<td>$C_{10}H_{15}OPS_2$</td>
<td>246.329</td>
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<td>$C_{10}H_5Cl_7$</td>
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<td>Heptachlor epoxide [1024–57–3]</td>
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<td>2,5-dichloro-4-iodophenyl $(RS)$-α-cyano-3-phenoxybenzyl $(RS)$-2-(4-chlorophenyl)-3-methylbutyrate</td>
<td>$C_8H_8Cl_2IO_3PS$</td>
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<td>Chlordecone</td>
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<td>Mirex [2385-85-5]</td>
<td>Dechlorane</td>
<td>1,1a,2,2,3a,4,5,5a,5b,6-dodeca-chlorooctahydro-1,3,4-metheno-1H-cyclobuta(cdp)entalene</td>
<td>$C_{10}Cl_{12}$</td>
<td>545.543</td>
<td>485</td>
<td>0.00031</td>
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<tr>
<td>Monocrotophos [6923-22-4]</td>
<td>Nuvacron, Azodrin</td>
<td>dimethyl (E)-1-methyl-2-(methyl carbamyl) vinyl phosphate</td>
<td>$C_{16}H_{14}NO_2P$</td>
<td>223.164</td>
<td>55</td>
<td>0.508</td>
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(Continued)
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<tr>
<th>Name</th>
<th>Synonym</th>
<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>Fugacity ratio, F at 25°C</th>
<th>pK_a</th>
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<tr>
<td>Naled [300–76–5]</td>
<td>Arthodibrom, Dibrom, Bromex, Bromchlorophos</td>
<td>1,2-dibromo-2,2-dichloroethyl dimethyl phosphate</td>
<td>C&lt;sub&gt;9&lt;/sub&gt;H&lt;sub&gt;6&lt;/sub&gt;Br&lt;sub&gt;2&lt;/sub&gt;ClO&lt;sub&gt;2&lt;/sub&gt;P</td>
<td>380.784</td>
<td>27</td>
<td>0.956</td>
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<td>Oxamyl [23135-22-0]</td>
<td>Vyteate</td>
<td>N&lt;sup&gt;1&lt;/sup&gt;-dimethyl-2-methylcarbamoyloxyimino-2-((methylthio)acetamine</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;S</td>
<td>219.261</td>
<td>109</td>
<td>0.150</td>
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<td>Parathion [56-38-2]</td>
<td>Foliod, Bladan, Niran</td>
<td>O&lt;sub&gt;2&lt;/sub&gt;O-diethyl O-4-nitrophenyl phosphorothioate</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;NO&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>291.261</td>
<td>6.1</td>
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<td>Parathion-methyl [298-00-0]</td>
<td>Dalf, Nitrox</td>
<td>O&lt;sub&gt;2&lt;/sub&gt;O-diethyl O-(p-nitrophenyl) phosphorothioate</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;NO&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>263.208</td>
<td>38</td>
<td>0.746</td>
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<td>Pentachlorophenol [87–86–5]</td>
<td>PCP</td>
<td>pentachlorophenol</td>
<td>C&lt;sub&gt;7&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt;Cl&lt;sub&gt;5&lt;/sub&gt;O</td>
<td>266.336</td>
<td>174</td>
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<td>Pentachlorophenol sodium salt (Pentacon)</td>
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<td>Permethrin [52645-53-1]</td>
<td>Ambush, Kafil, Picket, Prame</td>
<td>3-phenoxybenzyl(1RS,3RS;1RS,3RS)-3(2,2-dichlorovinyl)-2,2-dimethylcyclo-panecarboxylate</td>
<td>C&lt;sub&gt;21&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;Cl&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>391.288</td>
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<td>Phenthoate [2597-03-7]</td>
<td>Cidial, Eisan</td>
<td>ethyl 2-dimethoxythiophosphoryl-2-phenylacetate</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;17&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;PS&lt;sub&gt;2&lt;/sub&gt;</td>
<td>320.364</td>
<td>17-18</td>
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<td>Phorate [298-02-2]</td>
<td>Forsaat, Gramitox</td>
<td>O&lt;sub&gt;2&lt;/sub&gt;O-diethyl-S-(ethylthio)methyl phosphorodithioate</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;17&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>260.378</td>
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<td>Phosmet [732-11-6]</td>
<td>Imidan</td>
<td>S-[(1,3-dihydro-1,3-dioxo-2H-isodindol-2-yl)methyl]</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>317.321</td>
<td>72</td>
<td>0.346</td>
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<td>Phosphamidon [13171-21-6]</td>
<td>Dimecron</td>
<td>2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;19&lt;/sub&gt;ClNO&lt;sub&gt;2&lt;/sub&gt;P</td>
<td>299.689</td>
<td>–45</td>
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<td>Pirimicarb [23103-98-2]</td>
<td>Pirimor, Aphox</td>
<td>2-dimethylamino-5,6-dimethyl-pyrimidin-4-yl dimethylcarbamate</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;15&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>238.287</td>
<td>90.5</td>
<td>0.228</td>
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<td>Profenofos [41198-08-7]</td>
<td>Selecron</td>
<td>O&lt;sub&gt;4&lt;/sub&gt;-bromo-2-chlorophenyl O-ethyl S-propyl phosphorothioate</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;15&lt;/sub&gt;BrClO&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>373.631</td>
<td>liquid</td>
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<td>Propoxur [114-26-1]</td>
<td>Baygon</td>
<td>2-((1-Methylethoxy)phenol methyl carbamate</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;15&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>209.242</td>
<td>87</td>
<td>0.246</td>
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<td>Ronnel [299-84-3]</td>
<td>Fenchlorphos, Korlan, Etofene, Trolec, Trolef</td>
<td>O&lt;sub&gt;2&lt;/sub&gt;O-diethyl O-2,4,5-trichlorophenylphosphorothioate</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;15&lt;/sub&gt;ClO&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>321.546</td>
<td>41</td>
<td>0.697</td>
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<tr>
<td>Sulfotep [3689-24-5]</td>
<td>dithio, thiopen, ENT, Bladafum</td>
<td>O&lt;sub&gt;2&lt;/sub&gt;O,O'-tetraethyl dithiopyrophosphate</td>
<td>C&lt;sub&gt;8&lt;/sub&gt;H&lt;sub&gt;10&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;PS</td>
<td>322.320</td>
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<td>Terbacil [5902-51-2]</td>
<td>Sinbar, Turbacil</td>
<td>5-chloro-3-[(1,1-dimethyl)-6-methyl-2,4-((1H,3H)-pyrimidine-dione</td>
<td>C&lt;sub&gt;8&lt;/sub&gt;H&lt;sub&gt;13&lt;/sub&gt;ClN&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>216.664</td>
<td>176</td>
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<td>Insecticide</td>
<td>Brand Name(s)</td>
<td>Chemical Name</td>
<td>Molecular Formula</td>
<td>Molecular Weight</td>
<td>Form</td>
<td>Purity (ppm)</td>
<td></td>
</tr>
<tr>
<td>-------------</td>
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<td>---------------</td>
<td>-------------------</td>
<td>------------------</td>
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<tr>
<td>Terbufos [13071-79-9]</td>
<td>Contraven, Counter</td>
<td>S-tert-butylthiomethyl O,O-diethyl phosphorodithioate</td>
<td>C₉H₂₁O₂PS₃</td>
<td>288.431</td>
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<td>Terbufos sulfoxide</td>
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<td></td>
<td></td>
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<td></td>
<td></td>
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<tr>
<td>Terbufos sulfone</td>
<td></td>
<td></td>
<td>C₁₀H₁₉NO₄</td>
<td>331.407</td>
<td>65-80</td>
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<tr>
<td>Tetramethrin [7696-12-0]</td>
<td>Neo-Pynamin, phthalathrin</td>
<td>cyclohex-1-ene-1,2-dicarboximidomethyl (1RS,3RS;1RS,3SR)-2,2-dimethyl-3-methylprop-1-enyl)cyclopropanecarboxylate</td>
<td>C₁₉H₂₅NO₄</td>
<td>331.407</td>
<td>65-80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thiobencarb [28249-77-6]</td>
<td>Benthiocarb, Bolero, Saturno</td>
<td>S-(4-chlorophenyl)methyl diethyl-carbamothioate</td>
<td>C₁₂H₁₆ClNOS</td>
<td>257.779</td>
<td>1.7</td>
<td>1</td>
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<tr>
<td>Thiodicarb [59669-26-0]</td>
<td>Cicarbosulf, Larvin, Lepicron</td>
<td>dimethyl N,N′-thiobis(methylimino)-carbonyloxy bisethanimidiothioate</td>
<td>C₁₀H₁₈N₄O₄S₃</td>
<td>354.470</td>
<td>173</td>
<td>0.0353</td>
<td></td>
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<tr>
<td>Toxaphene [8001-35-2]</td>
<td>Camphechlor</td>
<td>chlorinated camphene (67–69% Cl content) - mixture</td>
<td>C₁₀H₁₀Cl₈</td>
<td>413.812</td>
<td>65-90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trichlorfon [52-68-6]</td>
<td>Tugon, Chlorophos, Dipterex, Neuguon</td>
<td>dimethyl 2,2,2-trichloro-1-hydroxy-ethylphosphonate</td>
<td>C₃H₇Cl₂O₂P</td>
<td>257.437</td>
<td>77</td>
<td>0.309</td>
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### TABLE 18.2.2
Summary of selected physical-chemical properties of insecticides at 25°C

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<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Solubility</th>
<th>Henry’s law constant</th>
<th>log K_{ow}</th>
<th>log K_{oc} reported</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>P^v/Pa</td>
<td>P^l/Pl</td>
<td>S/(g/m³)</td>
<td>C^v/(mol/m³)</td>
<td>C^l/(mol/m³)</td>
<td>H/(Pa·m³/mol)</td>
</tr>
<tr>
<td>Acephate</td>
<td>2.26 × 10^{-4}</td>
<td>8.96 × 10^{-4}</td>
<td>818000</td>
<td>4465</td>
<td>17710</td>
<td>–1</td>
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<tr>
<td>Aldicarb</td>
<td>0.004</td>
<td>0.0216</td>
<td>6000</td>
<td>31.54</td>
<td>170</td>
<td>1.1</td>
</tr>
<tr>
<td>Aldrin</td>
<td>0.005</td>
<td>0.0302</td>
<td>0.02</td>
<td>5.48 × 10^{-5}</td>
<td>3.31 × 10^{-4}</td>
<td>3.01</td>
</tr>
<tr>
<td>Aminocarb</td>
<td>0.00227</td>
<td>0.0109</td>
<td>915</td>
<td>4.39</td>
<td>21.1</td>
<td>1.73</td>
</tr>
<tr>
<td>Azinphos-methyl</td>
<td>3.0 × 10^{-5}</td>
<td>9.05 × 10^{-5}</td>
<td>30</td>
<td>0.0945</td>
<td>0.285</td>
<td>2.7</td>
</tr>
<tr>
<td>Bendiocarb</td>
<td>6.6 × 10^{-4}</td>
<td>7.21 × 10^{-3}</td>
<td>40</td>
<td>0.179</td>
<td>1.96</td>
<td>3.68 × 10^{-3}</td>
</tr>
<tr>
<td>Carbaryl</td>
<td>2.67 × 10^{-5}</td>
<td>3.83 × 10^{-4}</td>
<td>120</td>
<td>0.596</td>
<td>8.56</td>
<td>2.36</td>
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<tr>
<td>Carbofuran</td>
<td>8.0 × 10^{-5}</td>
<td>1.41 × 10^{-3}</td>
<td>351</td>
<td>1.59</td>
<td>28.0</td>
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<tr>
<td>Chlorfenvinphos</td>
<td>1.0 × 10^{-4}</td>
<td>1.0 × 10^{-4}</td>
<td>0.73</td>
<td>2.08 × 10^{-3}</td>
<td>3.07 × 10^{-3}</td>
<td>4.92</td>
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<tr>
<td>Chlorpyrifos</td>
<td>0.00227</td>
<td>3.34 × 10^{-4}</td>
<td>0.73</td>
<td>2.08 × 10^{-3}</td>
<td>3.07 × 10^{-3}</td>
<td>4.92</td>
</tr>
<tr>
<td>Chlorpyrifos-methyl</td>
<td>0.006</td>
<td>9.68 × 10^{-3}</td>
<td>4.76</td>
<td>0.0148</td>
<td>0.0238</td>
<td>0.0238</td>
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<tr>
<td>Crotosynaphos</td>
<td>0.0019</td>
<td>1.90 × 10^{-3}</td>
<td>1000</td>
<td>3.18</td>
<td>3.18</td>
<td>2.23</td>
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<tr>
<td>Cypermethrin#</td>
<td>1.87 × 10^{-7}</td>
<td>6.62 × 10^{-7}</td>
<td>0.004</td>
<td>9.61 × 10^{-6}</td>
<td>3.40 × 10^{-5}</td>
<td>6.6</td>
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<tr>
<td>α-cypermethrin</td>
<td>2.30 × 10^{-7}</td>
<td>8.21 × 10^{-7}</td>
<td>0.01</td>
<td>2.40 × 10^{-5}</td>
<td>8.41 × 10^{-5}</td>
<td>6.94*</td>
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<td>β-cypermethrin</td>
<td>1.80 × 10^{-7}</td>
<td>5.13 × 10^{-7}</td>
<td>0.0934</td>
<td>2.24 × 10^{-4}</td>
<td>6.4 × 10^{-4}</td>
<td>4.70*</td>
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<tr>
<td>ζ-cypermethrin</td>
<td>2.50 × 10^{-7}</td>
<td>2.50 × 10^{-7}</td>
<td>0.045</td>
<td>1.08 × 10^{-4}</td>
<td>1.08 × 10^{-4}</td>
<td>4.70*</td>
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<tr>
<td>DDD</td>
<td>1.30 × 10^{-4}</td>
<td>6.93 × 10^{-4}</td>
<td>0.05</td>
<td>1.56 × 10^{-4}</td>
<td>1.08 × 10^{-3}</td>
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<tr>
<td>DPE</td>
<td>2.0 × 10^{-4}</td>
<td>3.27 × 10^{-3}</td>
<td>0.10*</td>
<td>1.62 × 10^{-4}</td>
<td>1.08 × 10^{-3}</td>
<td>5.5</td>
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<tr>
<td>DDE</td>
<td>8.66 × 10^{-4}</td>
<td>3.72 × 10^{-3}</td>
<td>0.04</td>
<td>1.26 × 10^{-4}</td>
<td>5.40 × 10^{-4}</td>
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<td>DDT</td>
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<td>3.14 × 10^{-4}</td>
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<td>5.8</td>
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<td>DDD</td>
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<td>0.0055</td>
<td>1.55 × 10^{-5}</td>
<td>1.11 × 10^{-4}</td>
<td>6.19</td>
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<tr>
<td>DDT</td>
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<td>1.72 × 10^{-4}</td>
<td>0.026</td>
<td>7.33 × 10^{-5}</td>
<td>4.96 × 10^{-4}</td>
<td>4.37</td>
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<tr>
<td>Deltamethrin</td>
<td>1.0 × 10^{-5}</td>
<td>5.52 × 10^{-5}</td>
<td>0.002</td>
<td>3.96 × 10^{-6}</td>
<td>2.18 × 10^{-5}</td>
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<td>Demeton</td>
<td>0.0347</td>
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<td>60</td>
<td>0.232</td>
<td>0.232</td>
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<td>0.04</td>
<td>0.040</td>
<td>3300</td>
<td>14.3</td>
<td>14.3</td>
<td>2.79 × 10^{-3}</td>
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<tr>
<td>Insecticide</td>
<td>Toxicity 1</td>
<td>Toxicity 2</td>
<td>Toxicity 3</td>
<td>Toxicity 4</td>
<td>Toxicity 5</td>
<td>Toxicity 6</td>
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<td>------------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td>Diamidaphos</td>
<td>0.008</td>
<td>8.0 × 10⁻³</td>
<td>60</td>
<td>0.197</td>
<td>0.197</td>
<td>3.3</td>
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<td>Diazinon</td>
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<td>1.19 × 10⁻³</td>
<td>6.25</td>
<td>0.021</td>
<td>0.05</td>
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<td>0.25</td>
<td>7.93 × 10⁻⁴</td>
<td>7.93 × 10⁻⁴</td>
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<td>Dichlorvos</td>
<td>7.02</td>
<td>7.02</td>
<td>8000</td>
<td>36.20</td>
<td>36.20</td>
<td>1.45</td>
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<td>0.0213</td>
<td>1000000</td>
<td>4216</td>
<td>4216</td>
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<td>Dieldrin</td>
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<td>4.46 × 10⁻⁴</td>
<td>0.0142</td>
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<td>Diflubenzuron</td>
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<td>1.31 × 10⁻⁵</td>
<td>0.08</td>
<td>2.57 × 10⁻⁴</td>
<td>0.0281</td>
<td>0.78</td>
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<td>Dimethoate</td>
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<td>0.0061</td>
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<td>Endrin</td>
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<td>0.23</td>
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<td>30</td>
<td>0.108</td>
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<td>0.0199</td>
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<td>Fenvalerate</td>
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<td>0.085</td>
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<td>Heptachlor</td>
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<td>1.50 × 10⁻⁴</td>
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<td>Heptachlor epoxide</td>
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<td>Hexachlorocyclohexane</td>
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<td></td>
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<td>α-BHC</td>
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<td>0.10</td>
<td>1</td>
<td>3.44 × 10⁻³</td>
<td>0.115</td>
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<td>β-BHC</td>
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<td>0.1</td>
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<td>δ-BHC</td>
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<td>0.0268</td>
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<td>0.0275</td>
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<td>Ildofenphos</td>
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<td>4.4 × 10⁻⁴</td>
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<td>0.0521</td>
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<td>Kepone</td>
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<td>Leptophos</td>
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<td>0.439</td>
<td>0.439</td>
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<tr>
<td>Mecarbam</td>
<td>negligible</td>
<td>&lt; 1000</td>
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<td></td>
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<tr>
<td>Methamidophos</td>
<td>0.0023</td>
<td>3.59 × 10⁻³</td>
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<td>142</td>
<td>2210</td>
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(Continued)
<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Henry's law constant</th>
<th>log Koc reported</th>
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<tbody>
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<td></td>
<td>P^s/Pa</td>
<td>S/(g/m^3)</td>
<td>C^s/(mol/m^3)</td>
<td>H/(Pa·m^3/mol)</td>
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<td>Methiocarb</td>
<td>0.016*</td>
<td>30</td>
<td>0.133</td>
<td>2.92</td>
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<tr>
<td>Methomyl</td>
<td>0.0067</td>
<td>58000</td>
<td>358</td>
<td>0.60</td>
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<tr>
<td>Methoxychlor</td>
<td>0.00013</td>
<td>0.045*</td>
<td>1.30 × 10^-4</td>
<td>5.08</td>
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<td>Mevinphos</td>
<td>0.017</td>
<td>600000</td>
<td>268</td>
<td>0.5</td>
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<tr>
<td>Mirex</td>
<td>0.0001</td>
<td>6.5 × 10^-5</td>
<td>1.19 × 10^-7</td>
<td>6.9</td>
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<tr>
<td>Monocrotophos</td>
<td>0.00933</td>
<td>1000000</td>
<td>448</td>
<td>0.120</td>
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<td>Oxamyl</td>
<td>0.0306</td>
<td>282000</td>
<td>1290</td>
<td>2.48</td>
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<tr>
<td>Parathion</td>
<td>6.0 × 10^-4</td>
<td>12.4</td>
<td>0.0426</td>
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<tr>
<td>Parathion methyl</td>
<td>0.002</td>
<td>25</td>
<td>0.095</td>
<td>3.0</td>
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<tr>
<td>Pentachlorophenol</td>
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<td>14</td>
<td>0.053</td>
<td>0.79</td>
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<td>Permethrin</td>
<td>1.70 × 10^-6</td>
<td>0.006</td>
<td>1.53 × 10^-5</td>
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<tr>
<td>Phenthoate</td>
<td>3.5 × 10^-4</td>
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<td>0.0343</td>
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<td>Phorate</td>
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<td>22</td>
<td>0.0845</td>
<td>3.56</td>
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<td>Phosmet</td>
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<td>0.0788</td>
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<td>Phosphamidon</td>
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<td>2200</td>
<td>9.232</td>
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<td>Profenofos</td>
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<td>28</td>
<td>0.0749</td>
<td>1.60 × 10^-3</td>
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<td>Propoxur</td>
<td>1.70 × 10^-5</td>
<td>1800</td>
<td>8.603</td>
<td>1.98 × 10^-6</td>
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<tr>
<td>Pyrethrins</td>
<td>1.33 × 10^-6</td>
<td>0.001</td>
<td>3.05 × 10^-6</td>
<td>1.48</td>
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<tr>
<td>Ronnel (Fenchlorofos)</td>
<td>0.107</td>
<td>0.6</td>
<td>1.87 × 10^-3</td>
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<td>Sulfotep</td>
<td>0.0227</td>
<td>25</td>
<td>0.0776</td>
<td>0.293</td>
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<td>Terbacil</td>
<td>4.13 × 10^-5</td>
<td>710</td>
<td>3.276</td>
<td>1.26 × 10^-5</td>
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<td>Terbufos</td>
<td>0.0427</td>
<td>5</td>
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<td>0.0993</td>
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# isomer not specified

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.
### TABLE 18.2.3
Suggested half-life classes of insecticides 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>
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<td>Aldicarb</td>
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<td>6</td>
<td>8</td>
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<td>Aldrin</td>
<td>4</td>
<td>8</td>
<td>8</td>
<td>9</td>
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<tr>
<td>Carbaryl</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
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<tr>
<td>Carbofuran</td>
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<td>4</td>
<td>5</td>
<td>6</td>
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<tr>
<td>Chlordane</td>
<td>4</td>
<td>8</td>
<td>8</td>
<td>9</td>
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<td>Chloropyrifos</td>
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<td>4</td>
<td>4</td>
<td>6</td>
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<tr>
<td>DDE</td>
<td>4</td>
<td>7</td>
<td>8</td>
<td>9</td>
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<tr>
<td>p,p'-DDT</td>
<td>4</td>
<td>7</td>
<td>8</td>
<td>9</td>
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<td>Diazinon</td>
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<td>6</td>
<td>6</td>
<td>7</td>
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<tr>
<td>Dieldrin</td>
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<td>8</td>
<td>9</td>
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<td>Heptachlor</td>
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<td>5</td>
<td>6</td>
<td>7</td>
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<td>γ-HCH (lindane)</td>
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<td>8</td>
<td>9</td>
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<td>Malathion</td>
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<td>3</td>
<td>3</td>
<td>5</td>
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<tr>
<td>Methoxychlor</td>
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<td>7</td>
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<td>Mirex</td>
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<td>Parathion</td>
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<td>6</td>
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<tr>
<td>Parathion-methyl</td>
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<td>6</td>
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<tr>
<td>Propoxur</td>
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<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Toxaphene</td>
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<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
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<tr>
<td>1</td>
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<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>
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<tr>
<td>8</td>
<td>17000 (~ 2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>~ 5 years</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>
18.3 REFERENCES


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CLOGP (1986) Medchem Project of Pomona College, Claremont, California.


Dierberg, F.E., Pfeuffer, R.J. (1983) Fate of ethion in canals draining a Florida citrus grove.


Dorough, H.W., Marshall, T.C., Bryant, H.E. (1978) Fate of endosulfan in rats and toxicological conditions of apo lar...


Insecticides

4003


Hazardous Substances Data Bank (1989) National Library of Medicine, Toxicology Information Program.


Insecticides

4005


Insecticides


Martin, H. (1961) *Studies on the bioaccumulation and microbial degradation of 2,3,7,8-tetrachlorodibenz-


Sangster, J. (1993) LOGKOW Databank, Sangster Research Laboratory, Montreal, Quebec.


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- Penconazole .......................................................... 4086
- Propiconazole ........................................................ 4091
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19.1 LIST OF CHEMICALS AND DATA COMPILATIONS

19.1.1 Anilazine

Common Name: Anilazine
Synonym: Botrysan, Direz, Dyrene, Kemate, Triasyn, triazine, Zinochlor
Chemical Name: 2-chloro-\(N\)-(4,6-dichloro-1,3,5-triazin-2-yl)aniline; 2,4-dichloro-6-(o-chloro-anilino)-s-triazine; 4,6-dichloro-\(N\)-(2-chlorophenyl)-1,3,5-triazin-2-amine
Uses: as fungicide to control early and late blights of potatoes and tomatoes; anthracnose in cucurbits; leaf spot diseases in many crops; glume blotch of wheat; also used on vegetables, ornaments, berry fruits, melons, coffee and tobacco, etc.

CAS Registry No: 101-05-3
Molecular Formula: \(C_9H_5Cl_3N_4\)
Molecular Weight: 275.522
Melting Point (°C): 160 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C): 1.80 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm\(^3\)/mol):
\[\begin{align*}
252.8 & \text{ (calculated-Le Bas method at normal boiling point)} \\
153.1 & \text{ (calculated-density)}
\end{align*}\]
Dissociation Constant \(pK_a\):
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: 0.0474 (mp at 160°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
8.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8.00 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
negligible (20°C, Hartley & Kidd 1987)
8.20 × 10\(^{-7}\) (20°C, Worthing & Hance 1991; Tomlin 1994)

Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
2.82 × 10\(^{-5}\) (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
4.39 (calculated, Chiou 1981)
3.79 (calculated-CLOGP program, Biagi et al. 1991)
3.01 (20°C, Worthing & Hance 1991; Tomlin 1994)
3.88 (RP-HPLC-RT correlation, Saito et al. 1993)
1.91 (at pH 7, Milne 1995)
3.00 (selected, Hansch et al. 1995)

Bioconcentration Factor, log \(BCF\):
2.28 (calculated-S as per Kenaga 1980, this work)
Sorption Partition Coefficient, log $K_{OC}$:
- 3.00 (estimated-chemical structure, Lohninger 1994)
- 3.14 (calculated-S as per Kenaga 1980, this work)
- 3.00, 2.53, 3.30 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Hydrolysis: stable in neutral and slightly acidic media, $t_\frac{1}{2} = 730$ h at pH 4, $t_\frac{1}{2} = 790$ h at pH 7, $t_\frac{1}{2} = 22$ h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
- Soil: $t_\frac{1}{2} \sim 12$ h in damp soil (Hartley & Kidd 1987; Tomlin 1994);
- field $t_\frac{1}{2} = 1$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).
Biota:
19.1.2 **Benalaxyl**

![Chemical Structure](attachment://chemical_structure.png)

**Common Name:** Benalaxyl  
**Synonym:** Galben, M 9834, Tairel  
**Chemical Name:** methyl N phenylacetyl-N 2,6 xylyl-DL alaninate; methyl N 2,6 dimethylphenyl-N (phenylacetyl)-DL alaninate  
**CAS Registry No:** 71626-11-4  
**Uses:** as fungicide to control late blights of potatoes and tomatoes; downy mildews of hops, vines, lettuce, onions, soybeans and other crops; many diseases in flowers and ornamentals; and often used in combination with other fungicides, etc.

**Molecular Formula:** C₁₀H₁₃NO₃  
**Molecular Weight:** 325.402  
**Melting Point (°C):** 79  
(Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):** 1.27  
**Molar Volume (cm³/mol):** 390.8  
(calculated-Le Bas method at normal boiling point)  
**256.2**  
(calculated-density)  
**Dissociation Constant pKₐ:**  
**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:** 0.295 (mp at 79°C)  
**Water Solubility (g/m³ or mg/L at 25°C):** 37.0  
(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)  
37.0  
**Vapor Pressure (Pa at 25°C or as indicated):** 6.7 × 10⁻⁴  
(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
1.33 × 10⁻³  
**Henry’s Law Constant (Pa·m³/mol):** 0.0117  
(calculated-P/C, this work)  
**Octanol/Water Partition Coefficient, log Kₒw:** 3.40  
(Worthing & Hance 1991; Milne 1995)  
3.40  
(Tomlin 1994)  
3.40  
(selected, Hansch et al. 1995)  
3.24  
(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)  
**Bioconcentration Factor, log BCF:** 1.91  
(calculated-S as per Kenaga 1980, this work)  
**Sorption Partition Coefficient, log Kₒₑ:** 3.44–3.86  
(soil, Tomlin 1994)  
3.00  
(soil, estimated, Augustin-Beckers et al. 1994; Hornsby et al. 1996)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 86$ d at pH 9, 25°C, but stable in aqueous solutions at pH 4–9 (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil: $t_{1/2} = 20$–71 d in soil (Tomlin 1994);
field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:
19.1.3 **Benomyl**

![Chemical structure of Benomyl](image)

**Common Name:** Benomyl  
**Synonym:** Arilate, BBC, Benex, Benlate, Benosan, Fibenzo, Fundazol  
**Chemical Name:** methyl N-(1-butylcarbamoyl-2-benzimidazole)carbamate; methyl 1-(butyl-carbamoyl)benzimidazol-2-ylcarbamate; methyl 1-[(butylamino)carbonyl]-1H-benzimidazol-2-ylcarbamate  
**Uses:** as fungicide to control a wide range of diseases of fruit, nuts, vegetables, mushrooms, field crops, ornamentals, turf and trees; also provides secondary acaricidal control, principally as an ovicide, etc.  
**CAS Registry No:** 17804-35-2  
**Molecular Formula:** C_{14}H_{18}N_{4}O_{3}  
**Molecular Weight:** 290.318  
**Melting Point (°C):**  
- 140 (dec., Tomlin 1994)  
- dec (Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):**  
- 320.0 (calculated-Le Bas method at normal boiling point)  
**Molar Volume (cm³/mol):**  
- 320.0 (calculated-Le Bas method at normal boiling point)  
**Dissociation Constant pKₐ:**  
**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:** 0.0744 (mp at 140°C)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
- 3.8 (Austin et al. 1976; quoted, Kenaga 1980; Howard 1991)  
- 18.2, 4.0, 3.6, 2.8, 3.0, 1.9, 1.8, 8.8, 4.5 (pH 1, 3, 5.7, 8, 9, 10, 11, 12, room temperature, shake flask-HPLC/UV, Singh & Chiba 1985)  
- 2.8 (shake flask-HPLC/UV at pH 7, Singh & Chiba 1985; quoted, Howard 1991)  
- 2.0 (Hartley & Kidd 1987; Milne 1995)  
- 4.0 (pH 3–10, Worthing & Hance 1991)  
- 2.0 (stable only at pH 7, Montgomery 1993)  
- 4.0 (selected, Lohninger 1994)  
- 4.0 (pH 3–10, very soluble at pH 1, decomposes at pH 13, Tomlin 1994)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
- < 1.00 × 10⁻⁵ (20°C, Hartley & Kidd 1987)  
- < 4.90 × 10⁻⁶ (Tomlin 1994)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
- < 1.93 × 10⁻⁶ (calculated-P/C)  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
- 2.12 (20°C, shake flask-UV, Austin & Briggs 1976)  
- 2.42 (Rao & Davidson 1982; Hansch & Leo 1985; 1987)  
- 3.11 (Garten & Trabalka 1983; Travis & Arms 1988)  
- 2.12 (Hansch & Leo 1985)
2.42 (Sangster 1993)
1.40–3.11 (Montgomery 1993)
2.12 (recommended, Hansch et al. 1995)
1.33 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
2.46 (estimated-S, Kenaga 1980; quoted, Howard 1991)
–0.47 (vegetation, Popov & Shoeva 1974; Jalali & Anderson 1976)

Sorption Partition Coefficient, log KOC:
3.32 (estimated-S, Kenaga 1980; quoted, Howard 1991)
3.28 (soil, calculated, Montgomery 1993)
3.28 (selected, Lohninger 1994)
3.28 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
2.73, 1.92 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2} = 1.6$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Hydrolysis: very significant in water with $t_{1/2} < 1$ wk (Howard 1991).
Biodegradation:
Biotransformation:

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

Half-Lives in the Environment:
Air: estimated $t_{1/2} \sim 1.6$ h, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Surface water: $t_{1/2} = 2$ h (Tomlin 1994).
Groundwater:
Sediment:
Soil: degradation occurred within 15 d in unsterilized soil (Hine et al. 1969);
$\ t_{1/2} = 6–12$ months (Hartley & Kidd 1987);
field $t_{1/2} = 67$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$\ t_{1/2} = 19$ h in soil (Tomlin 1994).
Biota: $t_{1/2} = 3–7$ d on foliage (quoted, Montgomery 1993).
**19.1.4 BITERTANOL**

Common Name: Bitertanol  
Synonym: Baycor, Baymat, Biloxazol, Sibutol  
Chemical Name: 1-(biphenyl-4-yloxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)butan-2-ol; \( \beta \)-(1,1'-biphenyl-4-yloxy)-\( \alpha \)-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol  

Uses: as fungicide to control scab on apples and pears; rusts and powdery mildews on ornamentals; black spot on roses; and leaf spot and other diseases of vegetables, cucurbits, cereals, deciduous fruit, bananas, groundnuts, soy beans, etc.  
CAS Registry No: 70585-38-5 (diastereoisomer A), 55179-31-2 (diastereoisomer B)  
Molecular Formula: \( \text{C}_{20}\text{H}_{23}\text{N}_{3}\text{O}_{2} \)  
Molecular Weight: 337.415

Melting Point (°C):  
139.8 (diastereoisomer A, Hartley & Kidd 1987)  
146.3 (diastereoisomer B, Hartley & Kidd 1987)  
118.0 (eutectic mixture of the two diastereoisomers, Hartley & Kidd 1987; Worthing & Hance 1991)  
136.7 (diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)  
145.2 (diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Boiling Point (°C):  
Dissociation Constant pK\(_a\):  
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: 0.122 (eutectic mixture, mp at 118°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):  
5.0 (20°C, eutectic mixture; Hartley & Kidd 1987; Worthing & Hance 1991)  
2.9 (20°C, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)  
1.6 (20°C, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):  
1.0 \times 10^{-6} (20°C, Hartley & Kidd 1987)  
0.0038 (100°C, diastereoisomer A, Worthing & Hance 1991)  
0.0032 (100°C, diastereoisomer B, Worthing & Hance 1991)  
2.2 \times 10^{-10} (20°C, diastereoisomer A, Tomlin 1994)  
2.5 \times 10^{-10} (20°C, diastereoisomer B, Tomlin 1994)

Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):  
8.45 \times 10^{-5} (20°C, eutectic mixture, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):  
4.16 (Schreiber & Schönhe 1992)  
4.16 (selected, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
2.40 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
2.25 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis: stable in neutral, acidic and alkaline media, hydrolytic t_{1/2} > 1 yr at 25°C and pH 4, 7 and 9 (Tomlin 1994).
- Biodegradation: degradation in soil is rapid (Tomlin 1994).

Biotransformation:
- Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
- Surface water: environmental t_{1/2} = 1 month to 1 yr (Tomlin 1994).
19.1.5 **Bupirimate**

Common Name: Bupirimate  
Synonym: Nimrod, PP 588  
Chemical Name: 5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethylsulfamate; 5-butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate  
Uses: as fungicide to control powdery mildews of apples and pears, stone fruit, strawberries, gooseberries, vines, roses and other ornamentals, cucurbits, hops, beet, and other crops, etc.  
CAS Registry No: 41483-43-6  
Molecular Formula: C_{13}H_{24}N_{4}O_{3}S  
Molecular Weight: 316.419

Melting Point (°C):  
50–51  
(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Boiling Point (°C):  
Density (g/cm³ at 20°C):  
Molar Volume (cm³/mol):  
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:

Water Solubility (g/m³ or mg/L at 25°C):  
22.0  
(Martin & Worthing 1977)  
22.0  
(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
23.0  
(at pH 5.2, Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):  
6.7 × 10⁻⁵  
(20°C, Hartley & Kidd 1987; Worthing & Hance 1991)  
1.0 × 10⁻⁴  
(Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):  
9.64 × 10⁻³  
(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:  
2.70  
(shake flask, pH 7, Stevens et al. 1988)  
3.70  
(Worthing & Hance 1991)  
3.90  
(Tomlin 1994)  
2.70  
(selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:  
2.02  
(calculated-S, Kenaga 1980)  
2.56  
(calculated-K_{ow} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:  
2.90  
(calculated-S, Kenaga 1980)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

- **Volatileization:**
- **Photolysis:** rapidly decomposed by ultraviolet irradiation in aqueous solutions (Tomlin 1994).
- **Oxidation:**
- **Hydrolysis:** stable in dilute alkalis, but readily hydrolyzed by dilute acids (Tomlin 1994).
- **Biodegradation:**
- **Biotransformation:**

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

Half-Lives in the Environment:

- Soil: $t_\frac{1}{2} = 35–90$ d for nonsterile flooded or non-flooded soil, pH 5.1 to pH 7.3 (Tomlin 1994).
19.1.6 CAPTAN

Common Name: Captan
Synonym: Aacaptan, Amercide, Captab, Captaf, Captane, Captex, Flit 406, Glyodex 37-22, Malipur, Merpan, Orthocide, Pillarcap, Vondcaptan

Chemical Name: \(N\)-(trichloromethylthio)cyclohex-4-ene-1,2-dicarboximide; 1,2,3,6-tetrahydro-\(N\)-(trichloromethylthio)phthalimide; 3a,4,7,7a-tetrahydro-[(trichloromethyl)thio]-1\(H\)-isoindole-1,3(2\(H\))-dione

CAS Registry No: 133-06-2

Uses: as fungicide to control a wide range of fungal diseases; also used as seed treatment on maize, ornamentals, vegetables, oilseed rape, and other crops.

Molecular Formula: \(C_9H_8Cl_3NO_2S\)

Molecular Weight: 300.590

Melting Point (°C):
172.5 (Lide 2003)

Boiling Point (°C):
Density (g/cm³ at 20°C):
1.74 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):
250.5 (calculated-Le Bas method at normal boiling point)
172.8 (calculated-density)

Dissociation Constant \(pK_a\):  

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
44.35 (DSC method, Plato 1972)

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: 0.0357 (mp at 172.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
8.70 (colorimetric, Burchfield 1959)
< 0.5 (Martin & Worthing 1977)
0.50 (Briggs 1981)
3.30 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.50 (20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
1.44 (calculated, Patil 1994)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.0013 (Khan 1980)
< 0.0013 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0010 (20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
1.1 \times 10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
0.60 (20°C, calculated-P/C, Suntio et al. 1988)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 2.35 (Leo et al. 1971)
- 1.52 (Rao & Davidson 1980)
- 2.54 (shake flask-UV, Lord et al. 1980; Briggs 1981)
- 2.35 (Hansch & Leo 1985)
- 2.79 (Worthing & Hance 1991; Milne 1995)
- 2.35 (RP-HPLC-RT correlation, Saito et al. 1993)
- 2.60 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.35 (recommended, Sangster 1993)
- 2.35 (recommended, Hansch et al. 1995)
- 2.60 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- $> 2.96$ (estimated-S, Kenaga 1980a; quoted, Howard 1991)
- 2.67 (earthworms, Lord et al. 1980)
- 1.30 (activated sludge, Freitag et al. 1984, 1985)
- 1.30 (algae, Freitag et al. 1984, 85)
- 1.00 (golden ide, Freitag et al. 1985)
- 1.56 (regression-log $K_{OW}$, Hansch & Leo 1985)

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

- 2.30 (soil, converted from $K_{OM}$ multiplied by 1.724, Briggs 1981)
- 2.29 (Lyman et al. 1982; quoted, Howard 1991)
- 1.52 (estimated, Jury et al. 1987)
- 1.52 (screening model calculations, Jury et al. 1987b)
- 2.30 (soil, quoted exptl., Meylan et al. 1992)
- 2.94 (soil, calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
- 2.30 (selected, Lohninger 1994)
- 2.30 (soil, quoted or calculated-MCI $\chi$, Sabljic et al. 1995)

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

Vaporization:
- Photolysis: photolysis $t_{1/2} = 37$ min in isopropanol, $t_{1/2} = 420$ min in cyclohexene and $t_{1/2} = 380$ min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flößer-Müller 1990).
- Oxidation: photooxidation $t_{1/2} = 3.2–32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
- Hydrolysis: pseudo-first-order hydrolysis $t_{1/2} = 0.1$ d (Burchfield 1959; quoted, Freed 1976), $t_{1/2} = 1.8$ h, based on first-order rate constant $k = 6.5 \times 10^{-3}$ s$^{-1}$ at pH 7.1 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);
  - $t_{1/2} = 10.3$ h, based on first-order rate constant $k = 1.87 \times 10^{-5}$ s$^{-1}$ at pH 5.2 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);
  - $t_{1/2} = 10.5$ minutes, based on first-order rate constant $k = 1.10 \times 10^{-3}$ s$^{-1}$ at pH 8.3 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);
  - $t_{1/2} = 170$ min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);
  - over rate constant $k = 6.5 \times 10^{-3}$ s$^{-1}$ with $t_{1/2} = 3$ h at 25°C and pH 7 (Mabey & Mill 1978), $t_{1/2} = 7$ h in Lake Superior water at pH 7.6 and 12°C, $t_{1/2} = 1$ h at pH 7.6 and 25°C, $t_{1/2} = 40$ h at pH 6.7 and 12°C, and $t_{1/2} = 8$ h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).
- Biodegradation: unacclimated aqueous aerobic degradation $t_{1/2} = 48$–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991); unacclimated aqueous anaerobic degradation $t_{1/2} = 192$–5760 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991);
  - rate constant $k = 0.231$ d$^{-1}$ with a biodegradation $t_{1/2} = 3$ d in soil (Rao & Davidson 1980).

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

Air: $t_{1/2} = 2.6$ h and $1.4$ h for the vapor-phase reaction with photochemically produced hydroxyl radicals and ozone (Atkinson 1985; quoted, Howard 1991);
photooxidation $t_{1/2} = 3.2$–$32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be $<1$ d (Kelly et al. 1994).

Surface water: hydrolysis $t_{1/2} = 170$ min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

$t_{1/2} = 7$ h in Lake Superior water at pH 7.6 and 12°C, $t_{1/2} = 1$ h at pH 7.6 and 25°C, $t_{1/2} = 40$ h at pH 6.7 and 12°C, and $t_{1/2} = 8$ h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Groundwater: $t_{1/2} = 10.5$ min at pH 8.3 to $t_{1/2} = 10.3$ h at pH 5.2, based on first-order hydrolysis rate constants in surface waters (Wolfe et al. 1976; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 48$–$1440$ h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991);
rate constant $k = 0.231$ d$^{-1}$ with a biodegradation $t_{1/2} = 3$ d (Rao & Davidson 1980);
$t_{1/2} = 2.5$ d in soil (Halfon et al. 1996);
field $t_{1/2} = 2.5$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2} = 1$ d at pH 7.2 (Tomlin 1994).

Biota: biochemical $t_{1/2} = 3$ d from screening model calculations (Jury et al. 1987b).
19.1.7 CARBENDAZIM

Common Name: Carbendazim
Synonym: Bavistin, BCM, BMK, Carbendazime, Carbendazol, Carbendazym, G 665, Kemdazin, Mecarzole
Chemical Name: carbamic acid, methyl 1H-benzimidazol-2-yl, methyl ester; methyl benzimidazol-2-ylcarbamate; methyl 1H-benzimidazol-2-ylcarbamate
Uses: as fungicide for control of a wide range of fungal diseases in cereals, fruit, vines, hops, ornamentals, vegetables, rice, coffee, cotton, mushrooms, and other crops; also used by trunk injection to give some control of Dutch elm disease.
CAS Registry No: 10605-21-7
Molecular Formula: C₉H₉N₃O₂
Molecular Weight: 191.186
Melting Point (°C):
300 (dec, Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.45 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
194.8 (calculated-Le Bas method at normal boiling point)
131.9 (calculated-density)
Dissociation Constant pKₐ:
4.48 (Austin & Briggs 1976)
4.24 (Sangster 1993)
4.20 (Tomlin 1994)
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: 0.002 (mp at 300°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
8.0 (24°C at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
29, 8.0, 7.0 (24°C, at pH 4, 7, 8, Tomlin 1994)
8.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
6.50 × 10⁻⁸ (20°C, Hartley & Kidd 1987)
< 9.0 × 10⁻⁵ (20°C, Worthing & Hance 1991)
9.0 × 10⁻⁵, 1.5 × 10⁻⁴, 0.0013 (20, 25, 50°C, quoted, Tomlin 1994)
< 1.0 × 10⁻³ (20°C, quoted, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1.55 × 10⁻⁶ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_OW:
1.52 (shake flask, Austin & Briggs 1976)
1.40 (shake flask-UV, Lord et al. 1980)
1.34 (shake flask at pH 5, Barak et al. 1983)
Fungicides

1.56  (Worthing & Hance 1991; Milne 1995)
1.43  (recommended, Sangster 1993)
1.38, 1.505, 1.49  (pH 5, 7, 9, Tomlin 1994)
1.56, 1.77  (pH 6, 7, Tomlin 1994)
1.52  (recommended, Hansch et al. 1995)
1.80  (Pomona-database, Müller & Kördel 1996)
1.35  (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
2.28  (calculated-S, Kenaga 1980)
1.57  (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, log $K_{OC}$:
3.14  (soil, calculated-S, Kenaga 1980)
2.35  (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.30–2.40  (soil, Tomlin 1994)
2.35  (soil, calculated-MCl 1, Sabljic et al. 1995)
2.69  (soil, 20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.35; 2.25  (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.00, 2.09, 2.41, 2.28, 2.83  (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.318, 2.346, 2.091, 2.198  (second generation Eurosoils ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Hydrolysis: $t_{1/2} > 35$ d (pH 5 and 7 at 22°C, Worthing & Hance 1991);
slowly decomposed in alkaline solution, $t_{1/2} > 350$ d at pH 5, 7, 124 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} = 2$ and 25 months in water under aerobic and anaerobic conditions, respectively (Tomlin 1994).
Groundwater:
Sediment:
Soil: $t_{1/2} = 8–32$ d under outdoor conditions, decomposes with $t_{1/2} = 6–12$ months on bare soil, $t_{1/2} = 3$ to 6 months on turf (Tomlin 1994);
field $t_{1/2} = 120$ d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:
19.1.8 Carboxin

Common Name: Carboxin
Synonym: Carbathiin, D 735, Kemikar, Kisvax, Vitavax
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide; 2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathi-ine
CAS Registry No: 5234-68-4
Uses: as fungicide in seed treatment for control of seed diseases of barley, wheat, oats, rice, groundnuts, soybeans, cotton, vegetables, maize, and other crops, etc.
Molecular Formula: C_{12}H_{13}NO_{2}S
Molecular Weight: 235.302
Melting Point (°C):
91.5–92.5 (Spencer 1982; Harley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
98.0–100 (dimorphic, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
94 (Lide 2003)
Boiling Point (°C): 84
Density (g/cm³ at 20°C):
1.30 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Molar Volume (cm³/mol):
246.6 (calculated-Le Bas method at normal boiling point)
173.0 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₕus (kJ/mol):
22.175 (DSC method, Plato 1972)
Entropy of Fusion, ΔSₕus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕus = 56 J/mol K), F: 0.210 (mp at 94°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
170 (Martin & Worthing 1977)
170 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
199 (Worthing & Hance 1991; Tomlin 1994)
215 (calculated-group contribution fragmentation method, Kühe et al. 1995)
195 (selected, Lohninger 1994)
Vapor Pressure (Pa at 25°C or as indicated):
< 1.0 × 10⁻³ (20°C, Hartley & Kidd 1987)
2.5 × 10⁻⁵ (Worthing & Hance 1991; Tomlin 1994)
1.3 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.5 × 10⁻⁵ (20°C, Montgomery 1993)
Henry’s Law Constant (Pa·m³/mol at 25°C):
3.45 × 10⁻³ (calculated-P/C, Montgomery 1993)
1.57 × 10⁻³ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow}:
2.17 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)
2.18 (Tomlin 1994)
2.14 (selected, Hansch et al. 1995)
2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
Bioconcentration Factor, log BCF:
1.53       (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.41       (soil, calculated-S, Kenaga 1980)
2.41       (calculated, Montgomery 1993)
2.41       (estimated-chemical structure, Lohninger 1994)
2.57       (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives, t_{1/2}:
Volatilization:
   Photolysis: t_{1/2} < 3 h when exposed to light in aqueous solutions at pH 7 (Tomlin 1994).
Oxidation:
   Hydrolysis: t_{1/2} < 3 d when exposed to light (Montgomery 1993).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:

Half-Lives in the Environment:
Soil: t_{1/2} ~ 24 h (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
19.1.9 CHLORONEB

Common Name: Chloroneb
Synonym: Demesan; Tersan SP
Chemical Name: 1,4-dichloro-2,5-dimethoxybenzene
CAS Registry No: 2675-77-6
Uses: as fungicide applied to soil or used as seed treatment for control of seedling diseases of beans, cotton, soybeans, and beet; also used for control of snow mold (Typhula spp.) and Pythium blight on turf grass.
Molecular Formula: C₈H₈Cl₂O₂
Molecular Weight: 207.055

Melting Point (°C):
134 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.66 (Spencer 1982)
Molar Volume (cm³/mol):
200.4 (calculated-Le Bas method at normal boiling point)
124.8 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Vaporization, ΔHV (kJ/mol):
71.91 (Rordorf 1989)
Enthalpy of Fusion, ΔH₉ₐ₅ (kJ/mol):
30.54 (DSC method, Plato & Glasgow 1969)
29.1 (Rordorf 1989)
Entropy of Fusion, ΔS₉ₐ₅ (J/mol K):
72.0 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS₉ₐ₅ = 56 J/mol K), F: 0.0852 (mp at 134°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
8 (Martin & Worthing 1977; Spencer 1982)
8 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.40 (Spencer 1982)
0.40 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.017, 0.43, 6.90, 77.0, 630 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 16.452 − 5436/(T/K); measured range 32.5–135°C (solid, gas saturation-GC, Rordorf 1989)
log (P/Pa) = 12.303 − 3757.8/(T/K); measured range 136–151°C (liquid, gas saturation-GC, Rordorf 1989)
0.40 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₐ₉ₐ₅:
Bioconcentration Factor, log BCF:

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

3.06  (soil, Hamaker & Thompson 1972)
3.10  (soil, quoted exptl., Meylan et al. 1992)
2.36  (calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
3.22  (selected, Lohninger 1994)

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

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 24$ h (Worthing & Hance 1991);
field $t_{1/2} = 130$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).
19.1.10 CHLOROPICRIN

\[
\begin{align*}
\text{Cl} & \quad \text{Cl} \\
\text{Cl} & \quad \text{NO}_2 \\
\text{Cl} & \quad \text{Cl}
\end{align*}
\]

Common Name: Chloropicrin
Synonym: Acquinite, Nemax, Nitrochloroform, Picfume
Chemical Name: Trichloronitromethane
CAS Registry No: 76-06-2
Uses: fungicide/herbicide/insecticide/nematicide/rodenticide; used as a soil disinfectant for control of nematodes, soil insects, soil fungi, and weed seeds; also used for fumigation of stored grain to control insects and rodents, for glasshouse and mushroom-house fumigation, etc.

Molecular Formula: \( \text{CCl}_3\text{NO}_2 \)
Molecular Weight: 164.376

Melting Point (°C):
–64.0 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994; Lide 2003)

Boiling Point (°C):
112.4 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm³ at 20°C):
1.65659, 1.64756 (20°C, 25°C, Dreisbach 1961)
1.656 (20°C, Spencer 1982; Tomlin 1994)

Molar Volume (cm³/mol):
113.9 (calculated-Le Bas method at normal boiling point)
99.3 (calculated-density)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
11.68 (Dreisbach 1961)

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):
2270 (Martin & Worthing 1977; Kenaga 1980; Montgomery 1993; Lohninger 1994)
2270 (0°C, Spencer 1982; quoted, Howard 1991; Tomlin 1994)
2270, 1620 (0, 25°C, Hartley & Kidd 1987)
2300 (Davies & Lee 1987)
1621 (Howard 1991)
1620 (Tomlin 1994)

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.):
3174* (gas saturation, measured range 0–35°C, Baxter et al. 1920)
log (P/mmHg) = 8.2424 – 2045.1/(273 + t°C); temp range 0–35°C (gas saturation, Baxter et al. 1920)
2666* (20°C, summary of literature data, temp range –25.5 to 111.9°C, Stull 1947)
3324 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.03335 – 1369.70/(218.0 + t°C), temp range 28–176°C, (Antoine eq. for liquid state, Dreisbach 1961)
760, 3173 (0, 25°C, Spencer 1982)
3200 (Hartley & Kidd 1987)
3173 (Howard 1991)
2253, 3173, 4400 (20, 25, 30°C, Montgomery 1993)
Fungicides

Henry’s Law Constant (Pa·m³/mol at 25°C):
208.0 (Kawamoto & Urano 1989)

Octanol/Water Partition Coefficient, log K_{ow}:
1.03 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.09 (shake flask, Hansch & Leo 1987)
2.07 (Howard 1991)
1.03, 2.09 (Montgomery 1993)
2.09 (selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.90 (calculated, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
1.79 (calculated, Kenaga 1980)
1.91 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
1.79 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.79 (selected, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatileization: t½ = 4.3 h for evaporation from a body of water 1 m deep with a current of 1 m/s and a wind of 3 m/s (Howard 1991).
Oxidation:
Hydrolysis:
  stable in neutral aqueous solution and with a minimum t½ = 11 yr (Howard 1991).
Biodegradation: rate constant k(aerobic) = 1.5 d⁻¹ with t½ = 0.46 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.5 d⁻¹ with t½ = 0.46 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
  k(anaerobic) = 12 d⁻¹ and t½ = 0.058 d (corrigendum, Kawamoto & Urano 1991)
Biotransformation:
  Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:
Air: t½ = 20 d by photodegradation (Howard 1991).
Surface water: biodegradation t½ = 0.46 d at 20°C by aerobic activated sludge or anaerobic microorganisms (Kawamoto & Urano 1990)
volatilization t½ = 4.3 h from a model river and photodegradation t½ = 3 d in the surface layer of water (Howard 1991).
Groundwater:
Sediment:
Biota:
### TABLE 19.1.10.1
Reported vapor pressures of chloropicrin at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Log P (Pa)</th>
<th>Temperature (°C)</th>
<th>Log P (Pa)</th>
<th>Temperature (°C)</th>
<th>Log P (Pa)</th>
<th>Temperature (°C)</th>
<th>Log P (Pa)</th>
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<tbody>
<tr>
<td>-20</td>
<td>200</td>
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<td>20.0</td>
<td>2666</td>
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<td>111.9</td>
<td>101325</td>
<td></td>
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</tr>
</tbody>
</table>

**Equations:**

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

**References:**

- Baxter et al. 1920
- Stull 1947
- Spencer 1982
- Montgomery 1993

**Equation 2:**

\[
P / \text{mmHg} = \exp(A) \cdot \exp\left(\frac{B}{C - t/°C}\right) \quad \text{temp range 28–176°C}
\]

**FIGURE 19.1.10.1** Logarithm of vapor pressure versus reciprocal temperature for chloropicrin.
19.1.11 CHLOROTHALONIL

Common Name: Chlorothalonil
Synonym: Bravo, chlorthalonil, Daconil, DAC 2787, Exotherm, Forturf, Nopcocide N 96, TPN
Chemical Name: tetrachloroisophthalonitrile; 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; 2,4,5,6-tetrachloro-1,3-dicyanobenzene
CAS Registry No: 1897-45-6
Uses: fungicide, fumigant, soil insecticide
Molecular Formula: C₈Cl₄N₂
Molecular Weight: 265.911
Melting Point (°C):
  250 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C): 1.80 (Montgomery 1993; Tomlin 1994)
Molar Volume (cm³/mol):
  233.0 (calculated-Le Bas method at normal boiling point)
  147.7 (calculated-density)
Dissociation Constant pKₐ:
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: 0.0062 (mp at 250°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  0.60 (Martin & Worthing 1977; Kenaga 1980; Spencer 1982; Hartley & Kidd 1987; Worthing 1987, 1991)
  0.30 (Davies & Lee 1987)
  0.50 (calculated-group contribution fragmentation method, Kühne et al. 1995)
  0.60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
  0.90 (Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
  < 1.30 (40°C, Hartley & Kidd 1987; Worthing & Hance 1991)
  2.32 (Worthing & Walker 1987; quoted, Majewski & Capel 1995)
  0.133 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
  1.3 × 10⁻³ (40°C, Montgomery 1993)
  8.1 × 10⁻³ (selected, Brouwer et al. 1994)
  7.6 × 10⁻⁵ (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  576 (calculated-P/C as per Worthing 1987, Majewski & Capel 1995)
  0.0194 (20°C, Kawamoto & Urano 1989)
  0.0151 (20°C, calculated-bond contribution method, Meylan & Howard 1991)
  0.02 (Montgomery 1993)
Octanol/Water Partition Coefficient, log Kₐₜₜ:\n  0.14 (screening model calculations, Jury et al. 1987b)
2.64 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.64 (recommended, Sangster 1993)
2.89 (RP-HPLC-RT correlation, Saito et al. 1993)
2.90 (recommended, Hansch et al. 1995)
3.80 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
1.92 (calculated-S, Kenaga 1980)
1.66 (calculated-K<sub>ow</sub> as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K<sub>oc</sub>:
3.76 (soil, calculated, Kenaga 1980)
3.14 (soil, screening model calculations, Jury et al. 1987b)
3.14 (soil, Gustafson et al. 1989)
3.26 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
2.76, 3.14 (soil, Montgomery 1993)
3.00 (sand, quoted, Montgomery 1993)
3.14 (estimated-chemical structure, Lohninger 1994)
3.20, 4.15 (sand, silt, Tomlin 1994)
3.26 (soil, calculated-MCI χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, or Half-Lives, t<sub>1/2</sub>:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: biochemical t<sub>1/2</sub> = 70 d (Jury et al. 1987b);
first-order rate constants in biotic and abiotic shake-flask tests k = −0.0161 and −0.0155 d<sup>−1</sup> in nonsterile sediment/estuarine water and k = −0.00574 d<sup>−1</sup> in sterile sediment/estuarine water and k = −0.00355 and −0.00329 d<sup>−1</sup> in nonsterile estuarine water and k = −0.00283 d<sup>−1</sup> in sterile estuarine water both at Davis Bayou (Walker et al. 1988);
rate constant k(aerobic) = 1.7 d<sup>−1</sup> with t<sub>1/2</sub> = 0.41 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.7 d<sup>−1</sup> with t<sub>1/2</sub> = 0.41 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
Biotransformation:
Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:
Half-Lives in the Environment:
Air:
Surface water: biodegradation t<sub>1/2</sub> = 0.41 d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)
Groundwater:
Sediment:
Soil: t<sub>1/2</sub> = 70 d from screening model calculations (Jury et al. 1987b);
 t<sub>1/2</sub> ~ 1.5–3 months (Hartley & Kidd 1987; Worthing & Hance 1991);
 soil t<sub>1/2</sub> = 68 d (Gustafson 1989);
 field t<sub>1/2</sub> = 30 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
 t<sub>1/2</sub> = 4.1 d and 1.5–3 months (Montgomery 1993);
 t<sub>1/2</sub> = 5–35 d in aerobic and anaerobic soil studies and from a few hours to a few days in aerobic and anaerobic aquatic soil studies (Tomlin 1994).
Biota: biochemical t<sub>1/2</sub> = 70 d from screening model calculations (Jury et al. 1987b).
19.1.12 DAZOMET

Common Name: Dazomet
Synonym: tiazon, Mylone, Crag Fungicide 974, Salvo, Basamid, Fongosan
Chemical Name: 3,5-dimethyl-1,3,5-thiadiazinane-2-thione
Uses: soil fumigant, nematicide, fungicide, herbicide, insecticide
CAS Registry No: 533-74-4
Molecular Formula: C₅H₁₀N₂S₂
Molecular Weight: 162.276
Melting Point (°C):
    106 (Lide 2003)
Boiling Point (°C):
Density (g/cm³): 1.37 (Montgomery 1993; Tomlin 1994)
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/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: 0.160 (mp at 106°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    1200 (Spencer 1982)
Vapor Pressure (Pa at 25°C or as indicated):
    4.0 × 10⁻⁴, 3.73 × 10⁻⁴ (20°C, quoted, Augustijn-Beckers et al. 1994)
    4.0 × 10⁻⁴ (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
    2.03 (20°C, calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log Kₐw:
    0.15 (Montgomery 1993)
    1.40 (at pH 7, Tomlin 1994)
Octanol/Air Partition Coefficient, log Kₐₐ:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₒₑ:
    0.48 (calculated, Montgomery 1993)
    −0.046 at pH 9, 0.778 (quoted values, Augustijn-Beckers et al. 1994)
    1.0 (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Environmental Fate Rate Constants, k, and Half-Lives, t₁/₂:
Half-Lives in the Environment:
19.1.13 DICHLONE

Common Name: Dichlone
Synonym: Algistat, Compound 604, Ent 3776, Phygon, Quintar, Sanquinon
Chemical Name: 2,3-dichloro-1,4-naphthoquinone; 2,3-dichloro-1,4-naphthalenedione
CAS Registry No: 117-80-6
Uses: fungicide/algicide; as fungicide for control of blossom blights, scab on apples and pears and brown spot on stone fruit, etc.; also used to control blue-green algae in ponds, lakes, and swimming pools.
Molecular Formula: C<sub>10</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub>
Molecular Weight: 227.044
Melting Point (°C):
195 (Lide 2003)
Boiling Point (°C):
275 (at 2 mmHg, Hartley & Kidd 1987; Howard 1991; Montgomery 1993)
Density (g/cm<sup>3</sup> at 20°C):
196.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK<sub>a</sub>
Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):
78.30 (Rordorf 1989)
Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):
27.0 (Rordorf 1989)
Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):
58 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0215 (mp at 195°C)
Water Solubility (g/m<sup>3</sup> or mg/L at 25°C as indicated):
0.10 (Kenaga 1980)
8.00 (20°C, Hodnett et al. 1983)
0.10 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1.00 (Montgomery 1993)
0.10 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
3.30 × 10<sup>–4</sup>, 8.80 × 10<sup>–3</sup>, 0.15, 1.70, 14.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P<sub>v</sub>/Pa) = 14.965 – 5500.9/(T/K); measured range 40.4–191°C (solid, gas saturation-GC, Rordorf 1989)
log (P<sub>v</sub>/Pa) = 13.396 – 4803.6/(T/K); measured range 40.4–191°C (liquid, gas saturation-GC, Rordorf 1989)
1.47 × 10<sup>–4</sup> (calculated from S and Henry’s law constant, Howard 1991)
Henry’s Law Constant (Pa·m<sup>3</sup>/mol at 25°C):
6.51 × 10<sup>–5</sup> (Hine & Mookerjee 1975)
Octanol/Water Partition Coefficient, log K<sub>ow</sub>:
3.16 (estimated, Hodnett et al. 1983)
5.62 (calculated, Montgomery 1993)
Bioconcentration Factor, log BCF:
3.35 (estimated-S, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log KOC:
4.19 (estimated-S, Kenaga 1980; quoted, Howard 1991)
4.19 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t1/2:
Volatilization:
Photolysis:
Oxidation: estimated photooxidation \( t_{1/2} = 3.87 \) d in air, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Hydrolysis: \( t_{1/2} = 5 \) d at pH 7 (Howard 1991).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

Half-Lives in the Environment:
Air: estimated \( t_{1/2} = 3.87 \) d, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Surface water:
Groundwater:
Sediment:
Soil: \( t_{1/2} = 1 \) d in moist and slightly under three months in dry silt loam soil at pH 6.2–6.4 and 29°C, respectively (Burchfield 1959; quoted, Howard 1991);
field \( t_{1/2} = 10 \) d (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:
19.1.14 DICOFOL

Common Name: Dicofol
Synonym: kelthane, kelthan
Chemical Name: 2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethenol, 4-chloro-α-(4-chlorophenyl)-α-(trichloromethyl)-benzenemethanol
Uses: acaricide
CAS Registry No: 115-32-2
Molecular Formula: C_{14}H_{9}Cl_{5}O
Molecular Weight: 370.485
Melting Point (°C):
77.5 (Lide 2003)
Boiling Point (°C):
180 (0.1 mmHg, Hartley & Kidd 1987)
193 (360 mmHg, tech., Tomlin 1994)
Density (g/cm³): 1.45 (Worthing & Walker 1987; Tomlin 1994)
Acid Dissociation Constant, pK_a:

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
104.0 (Rordorf 1989)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
19.8 (Rordorf 1989)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
57 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.305 (mp at 77.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1.32 (generator column-GC/ECD, Weil et al. 1974)
1.20 (24°C, 99% purity, Verschueren 1983)
0.80 (20°C, in distilled water, Verschueren 1983)
0.80 (selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.80 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.40 \times 10^{-5}, 1.20 \times 10^{-3}, 0.032, 0.56, 68.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_v/P_a) = 17.084 – 6470.1/(T/K); measured range 85.5–145°C (solid, gas saturation-GC, Rordorf 1989)
log (P_v/P_a) = 14.104 – 5354.8/(T/K); measured range 85.5–145°C (liquid, gas saturation-GC, Rordorf 1989)
5.33 \times 10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)
5.30 \times 10^{-5} (tech., Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
5.66 \times 10^{-5} (calculated-bond contribution method, Howard 1991)

Octanol/Water Partition Coefficient, log $K_{ow}$:
3.54 (Rao & Davidson 1980)
3.54 (Nigg et al. 1986)
4.28 (Tomlin 1994)
3.54 (Hansch & Leo 1987; quoted, Sangster 1993)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_B$:
- 4.18–4.27  (fathead minnow, Howard 1991)
- 3.98–4.16  (in presence of suspended clay, Howard 1991)
- 2.75, 3.54  (calculated-S, calculated-$K_{OW}$, Howard 1991)

Sorption Partition Coefficient, log $K_{OC}$:
- 3.60, 3.30  (estimated-S, calculated-$K_{OW}$, Howard 1991)
- 3.46–3.91  (range of reported data, Wauchope et al. 1992)
- 3.70       (soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.92, 3.91, 3.79, 3.77  (sand, sandy loam, silty loam, clay loam, Tomlin 1994)

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

Vaporization:
Photolysis: direct photolysis $t_{1/2} = 2.92$ d in the atmosphere for reaction with OH radicals; $t_{1/2} = 6$ d for exposure of thin film of dicofol to sunlight at 300 nm (Howard 1991).

Photooxidation:
Hydrolysis: $t_{1/2} = 60$ min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L (Verschueren 1983); stable to acids, but unstable in alkaline media, $t_{1/2} = 85$ d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).
Biodegradation: degradation in anaerobic sewage to 4,4'-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983).

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

Half-Lives in the Environment:

Air: vapor phase $t_{1/2} \sim 2.92$ s life in the atmosphere for reaction with OH radicals (estimated, Howard 1991)

Surface water: hydrolysis $t_{1/2} = 60$ min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L; degradation in anaerobic sewage to 4,4'-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983)

Aqueous photodegradation $t_{1/2} = 1–4$ d at pH 5 in sensitized conditions and $t_{1/2} = 15–93$ d in unsensitized conditions; stable to acids, but unstable in alkaline media, $t_{1/2} = 85$ d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).

Ground water:

Sediment:

Soil: field $t_{1/2} = 45$ d (Wauchope et al. 1992; Hornsby et al. 1996);

soil photodegradation $t_{1/2} = 30$ d in silt loam, soil metabolism $t_{1/2} = 61$ d under aerobic conditions and $t_{1/2} = 16$ d under anaerobic conditions in silt loam; field dissipation $t_{1/2} = 60–100$ d (Tomlin 1994).
19.1.15 DITHIANON

Common Name: Dithianon
Synonym: Delan, Delan-Col
Chemical Name: 2,3-dicyano-1,4-dithiaanthraquinone; 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-p-dithin-2,3-dicarboxy-nitrile
CAS Registry No: 3347-22-6
Uses: as fungicide for control of many foliar diseases.
Molecular Formula: C_{14}H_{4}N_{2}O_{2}S_{2}
Molecular Weight: 296.324
Melting Point (°C): 220 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
   1.580 (Tomlin 1994)
Molar Volume (cm³/mol):
   264.0 (calculated-Le Bas method at normal boiling point)
   187.6 (calculated-density)
Dissociation Constant pKₐ:
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: 0.0122 (mp at 220°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   0.50 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Vapor Pressure (Pa at 25°C):
   6.6 × 10⁻⁵ (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   0.0391 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{OW}:
   2.84 (Worthing & Hance 1991)
   3.20 (Tomlin 1994)
   2.84 (selected, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
   2.96 (calculated-S per Kenaga 1980, this work)
Sorption Partition Coefficient, log K_{OC}:
   3.81 (soil, calculated-S per Kenaga 1980, this work)
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
   Volatilization:
      Photolysis: t_{1/2} = 19 h when exposed to artificial sunlight in 0.1 mg/L aqueous solution (Tomlin 1994).
      Oxidation:
      Hydrolysis: t_{1/2} = 12.2 h at pH 7 (Tomlin 1994).
Fungicides

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:
Surface water: hydrolysis $t_{1/2} = 12.2$ h at pH 7 and photolytic $t_{1/2} = 19$ h when exposed to artificial sunlight in 0.1 mg/L aqueous solutions (Tomlin 1994).
19.1.16 EDifenphos

Common Name: Edifenphos
Synonym: EDDP, Hinosan, edifenfos
Chemical Name: O-ethyl S,S-diphenyl phosphorodithioate
CAS Registry No: 17109-49-8
Uses: as fungicide for control of blast and blight diseases in rice, etc.
Molecular Formula: C₁₄H₁₅O₂PS₂
Molecular Weight: 310.371
Melting Point (°C):
  −25 (Tomlin 1994)
Boiling Point (°C):
  154 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)
Density (g/cm³ at 20°C):
  1.230 (Hartley & Kidd 1987; Worthing & Hance 1991)
  1.251 (Tomlin 1994)
Molar Volume (cm³/mol):
  250.5 (calculated from density)
Dissociation Constant pKₐ:
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  56.0 (20°C, Hartley & Kidd 1987; Tomlin 1994)
  insoluble (Worthing & Hance 1991)
Vapor Pressure (Pa at 25°C or as indicated):
  0.013 (20°C, Hartley & Kidd 1987)
  0.013 (20°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  0.0721 (20°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₐw:
  3.48 (RP-HPLC-RT correlation, Saito et al. 1993)
  4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)
Bioconcentration Factor, log BCF:
  1.81 (calculated-S as per Kenaga 1980, this work)
Sorption Partition Coefficient, log KₐOC:
  2.68 (calculated-S as per Kenaga 1980, this work)
Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:
  Hydrolysis: hydrolyzed by strong acids and alkalis, at 25°C, t₁/₂ = 19 d at pH 7 and t₁/₂ = 2 d at pH 9 (Tomlin 1994).
  Air:
  Surface water: hydrolysis t₁/₂ = 19 d at pH 7 and t₁/₂ = 2 d at pH 9 (Tomlin 1994).
Groundwater:
Sediment:
Soil: half-life in soil in the range of few days to a few weeks (Tomlin 1994).

Biota:
19.1.17 ETRIDIAZOLE

Common Name: Etridiazole
Synonym: Aaterra, Banrot, Dwell, Echlowezol, ETCMTD, Ethazole, ETMT, Koban, MF-344, OM 2425, Pansoil, Terracoat, Terrazole, Truban
Chemical Name: 5-ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole; ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether
Uses: as fungicide for control of Phytophthora and Pythium spp. in cotton, ornamentals, vegetables, groundnuts, cucurbits, tomatoes, and other crops; also used as a nitrification inhibitor in maize, cotton and wheat.
CAS Registry No: 2593-15-9
Molecular Formula: C₅H₅Cl₃N₂OS
Molecular Weight: 247.530
Melting Point (°C):
19.9 (Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
95.0 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm³ at 20°C):
1.503 (25°C, Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm³/mol):
219.0 (calculated-Le Bas method at normal boiling point)
164.7 (calculated-density)
Dissociation Constant pKₐ:
2.77 (Tomlin 1994)
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):
50.0 (Hartley Kidd 1987; Worthing & Hance 1991; Milne 1995; selected, Lohninger 1994)
50.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
0.013 (20°C, Hartley & Kidd 1987)
0.013 (rm. temp., Worthing & Hance 1991)
0.013 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0644 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K_{ow}:
2.48–2.60 (Worthing & Hance 1991; Milne 1995)
3.36 (Tomlin 1994)
2.55 (selected, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.83 (calculated-S as per Kenaga 1980, this work)
1.22 (calculated-K_{ow} as per Kenaga 1980, this work)
Sorption Partition Coefficient, log K_{OC}:
0.725 (sandy soil, Worthing & Hance 1991)
0.149 (silt loam, Worthing & Hance 1991)

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

Volatileization:
Photolysis:
Oxidation:
Hydrolysis: $t_{1/2} = 103$ d at pH 6 (Worthing & Hance 1991);
$t_{1/2} = 12$ d at pH 6, 45°C, $t_{1/2} = 103$ d at pH 6, 25°C (Tomlin 1994).

Biodegradation: soil $t_{1/2} = 9.5$ d under aerobic conditions and $t_{1/2} = 3$ d under anaerobic conditions (Tomlin 1994).
Biotransformation:

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

Half-Lives in the Environment:
Soil: $t_{1/2} = 9.5$ d under aerobic, $t_{1/2} = 3$ d under anaerobic conditions, field dissipation $t_{1/2} = 1$ wk in sandy clay loam (Tomlin 1994);
field $t_{1/2} = 103$ d (20–25°C, selected, Hornsby et al. 1996).
19.1.18 Fenarimol

Common Name: Fenarimol
Synonym: Bloc, EL-222, Rimidin, Rubigan
Chemical Name: (±)-2,4′-dichloro-α-(pyrimidin-5-yl)benzhydryl alcohol; α-(2-chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol
CAS Registry No: 60168-88-9
Uses: as fungicide for control of powdery mildews in pome fruit, strawberries, vines, cucurbits, roses, and beet; also for control of scab on pome fruit, brown patch and snow mold of turf.
Molecular Formula: C₁₇H₁₂Cl₂N₂O
Molecular Weight: 331.195
Melting Point (°C):
  118 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  338.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
  2.58 (Sangster 1993)
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: 0.122 (mp at 118°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  13.7 (Martin & Worthing 1977)
  13.7 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
  14.0 (selected, Lohninger 1994)
Vapor Pressure (Pa at 25°C or as indicated):
  < 1.3 × 10⁻⁵ (Hartley & Kidd 1987)
  1.30 × 10⁻³ (Worthing & Hance 1991)
  6.5 × 10⁻⁵ (vapor pressure balance, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  6.93 × 10⁻⁴ (20–25°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₖₐw:
  0.67 (shake flask, at pH 5.3, Martin & Edgington 1981)
  −1.59 (shake flask-UV at pH 5, Barak et al. 1983)
  3.70 (Stevens et al. 1988)
  3.60 (shake flask-HPLC, Bateman et al. 1990)
  3.69 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
  3.60 (selected, Hansch et al. 1995)
  3.61 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
Bioconcentration Factor, log BCF:
2.16 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log $K_{OC}$:
3.01 (calculated-S, Kenaga 1980)
0.176–1.08 (soil, Tomlin 1994)
2.78 (estimated-chemical structure, Lohninger 1994)

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

Volatileization:
Photolysis: decomposed readily by sunlight (Tomlin 1994).

Oxidation:
Hydrolysis: $t_{1/2} = 28$ d at 52°C and pH 3, 6 and 9 (Tomlin 1994).
Biodegradation: $t_{1/2} > 365$ d under aerobic conditions in soil, and microbial degradation is accelerated by light (Tomlin 1994).

Biotransformation:

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

Half-Lives in the Environment:
Soil: $t_{1/2} > 365$ d under aerobic conditions in soil (28% sand, 14.7% clay, 57.3% silt and pH 6 (Tomlin 1994)
**FENFURAM**

![Chemical Structure]

**Common Name:** Fenfuram  
**Synonym:** Panoram  
**Chemical Name:** 2-methylfuran-3-carboxanilide; 2-methyl-3-furanilide; 2-methyl-N-phenyl-3-furancarboxamide  
**CAS Registry No:** 24691-80-3  
**Uses:** as fungicide for control of bunts and smuts (*Tilletie* and *Ustilago* spp.) in cereals, when applied as a seed treatment.  
**Molecular Formula:** C$_{12}$H$_{11}$NO$_2$  
**Molecular Weight:** 201.221  
**Melting Point (°C):** 109–110 (Worthing & Hance 1991)  
**Boiling Point (°C):**  
**Density (g/cm$^3$ at 20°C):** 1.36 (Worthing & Hance 1991)  
**Molar Volume (cm$^3$/mol):**  
- 217.1 (calculated-Le Bas method at normal boiling point)  
- 148.0 (calculated-density)  
**Dissociation Constant pK$_a$:**  
**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 or as indicated):**  
- 100 (Martin & Worthing 1977; Kenaga 1980)  
- 100 (20–25°C, selected, Hornsby et al. 1996)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
- $2.0 \times 10^{-5}$ (20°C, Hartley & Kidd 1987)  
- $2.0 \times 10^{-5}$ (extrapolated to 20°C, Worthing & Hance 1991; Tomlin 1994)  
- $2.0 \times 10^{-5}$ (20–25°C, selected, Hornsby et al. 1996)  
**Henry’s Law Constant (Pa-m$^3$/mol):**  
**Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:**  
**Bioconcentration Factor, log BCF:**  
- 1.66 (calculated-S, Kenaga 1980)  
**Sorption Partition Coefficient, log $K_{\text{OC}}$:**  
- 2.54 (calculated-S, Kenaga 1980)  
- 2.48 (20–25°C, estimated, Hornsby et al. 1996)  
**Environmental Fate Rate Constants, k, or Half-Lives, $t_{\frac{1}{2}}$:**  
- **Hydrolysis:** stable in neutral media, but hydrolyzed by strong acids and alkalis (Tomlin 1994).  
- **Half-Lives in the Environment:**  
  - Soil: $t_{\frac{1}{2}} \approx 42$ d (Hartley & Kidd 1987; Tomlin 1994);  
  - field $t_{\frac{1}{2}} = 42$ d (20–25°C, selected, Hornsby et al. 1996).
19.1.20 FOLPET

Common Name: Folpet
Synonym: ENT-26539, Faltan, Folpan, Folpel, Ftal, Fungitrol, Orthophaltan, Phaltan, Spolacid, Thiophal, Vinicoll
Chemical Name: N-(trichloromethylthio)phthalimide; 2-[(trichloromethylthio)-1H-isooindole-1,3(2H)-dione
CAS Registry No: 133-07-3
Uses: fungicide for control of downy/powdery mildews, leaf spot diseases, etc.
Molecular Formula: C₉H₄Cl₃NO₂S
Molecular Weight: 296.558
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
246.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
8.50 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0323 (mp at 177°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
1.0 (Martin & Worthing 1977)
1.0 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
< 0.0013 (20°C, Hartley & Kidd 1987)
0.0013 (20°C, Worthing & Hance 1991; Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
3.63 (shake flask-UV, Briggs 1981)
2.85 (selected, Yoshioka et al. 1986)
2.85 (shake flask, log P database, Hansch & Leo 1987)
2.85 (recommended, Sangster 1993)
3.11 (Tomlin 1994)
2.85 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
1.91 (calculated-S, Kenaga 1980)
3.32 (earthworms, Lord et al. 1980)
Sorption Partition Coefficient, log K_{OC}:
1.78 (calculated-S, Kenaga 1980)
3.03 (reported as log K_{OM}, Briggs 1981)
3.27, 2.16 (soil, quoted exptl., calculated-fragment contribution method, Meylan et al. 1992)
3.27 (soil, calculated-MCI ¹χ, Sabljic et al. 1995)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

**Vaporization:**
Photolysis: $t_{1/2} = 101$ min in isopropanol, $t_{1/2} = 144$ min in cyclohexene and $t_{1/2} = 1620$ min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flößer-Müller 1990).

**Oxidation:**
Hydrolysis: hydrolyze at pH 7 with rates similar to captan, i.e., first-order rate constant $k = 6.5 \times 10^{-5}$ s$^{-1}$ with $t_{1/2} = 2.96$ h in a phosphate buffer solution at pH 7.07 and 28°C (Wolfe et al. 1976).

**Biodegradation:**

**Biotransformation:**

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

Half-Lives in the Environment:

**Air:**
Surface water: $t_{1/2} = 4.3$ d (Tomlin 1994).

**Groundwater:**

**Sediment:**

**Soil:** $t_{1/2} = 4.3$ d (Tomlin 1994).

**Biota:**
19.1.21 **FORMALDEHYDE**

![Formaldehyde structure](image)

**Common Name:** Formaldehyde  
**Synonym:** formalin, methanal, oxomethane  
**Chemical Name:** formaldehyde  
**Uses:** fungicide/bactericide; used as a soil sterilant in mushroom houses and other areas; also used as a silage preservative.

**CAS Registry No:** 50-00-0  
**Molecular Formula:** HCHO  
**Molecular Weight:** 30.026

- **Melting Point (°C):** –92 (Weast 1982–83; Dean 1985; Lide 2003)
- **Boiling Point (°C):** –19.1 (Lide 2003)
- **Density (g/cm³):**  
  - 0.815 (Weast 1982–83)
  - 0.815 (–20°C, Verschueren 1983; Dean 1985)

**Acid Dissociation Constant, pKₐ:**

**Molar Volume (cm³/mol):** 29.6 (calculated-Le Bas method at normal boiling point)

**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:** 1.0

**Water Solubility (g/m³ or mg/L at 25°C):**  
- 1,220,000 (Dean 1985)  
  - very soluble, up to 55% (Howard 1989)

**Vapor Pressure (Pa at 25°C or as indicated):**  
- 1333 (–88°C, Verschueren 1983)
- 451030 (> 1 atmospheric pressure, Howard 1989)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
- 0.0331 (Dong et al. 1986)
- 0.0169 (Gaffney et al. 1987)
- 0.0298 (gas stripping-HPLC, Zhou & Mopper 1990)

**Octanol/Water Partition Coefficient, log Kᵦₑ:**

- –0.75 (calculated-f const. per Rekker 1977, Deneer et al. 1988)
- 0.00 (calculated, Verschueren 1983)
- 0.35 (Howard 1989)
- 0.35 (recommended, Sangster 1989, 1993)

**Bioconcentration Factor, log BCF:**

- no bioconcentration in fish and shrimp observed (Howard 1989)

**Sorption Partition Coefficient, log Kᵦₑ:**

- 0.365 (estimated-S as per Kenaga 1980, this work)

**Environmental Fate Rate Constants, k, and Half-Lives, tᵢₜ:**

- **Volutilization:** sunlight photolysis tᵢₜ = 1.25–6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991).
Oxidation: rate constant \( k = 3.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor-phase reaction with NO\(_3\) radicals in the atmosphere at \( (298 \pm 1) \text{ K} \) (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986); rate constant \( k = 4.50 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor-phase reaction with HO\(_2\) radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986); rate constant \( k = 111.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor-phase reaction with OH radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986); atmospheric photooxidation \( t_{1/2} = 7.13–71.3 \text{ h} \), based on measured rate constant for the vapor-phase reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991); aqueous photooxidation \( t_{1/2} = 4,813–190,000 \text{ h} \), based on measured rate constant for the reaction with OH radicals in water (Dorfman & Adams 1973; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic \( t_{1/2} = 24–168 \text{ h} \), based on unacclimated aqueous aerobic biodegradation screening test data (Gellman & Heukelekian 1950; Heukelekian & Rand 1955; quoted, Howard et al. 1991); aqueous anaerobic \( t_{1/2} = 96–672 \text{ h} \), based on 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 Environmental Compartments:

Air: photooxidation \( t_{1/2} = 7.13–71.3 \text{ h} \), based on measured rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991); \( t_{1/2} = 1.26–6.0 \text{ h} \), based on photolysis half-life in air (Howard et al. 1991).

Surface water: \( t_{1/2} = 24–168 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: \( t_{1/2} = 48–336 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} = 24–168 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
19.1.22 Hexachlorobenzene

(See also Chapter 6. Chlorobenzenes and other Halogenated Mononuclear Aromatics)

Common Name: Hexachlorobenzene
Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride
Chemical Name: hexachlorobenzene
Uses: as fungicide for seed treatment to control common bunt and dwarf bunt of wheat.
CAS Registry No: 118-74-1
Molecular Formula: C₆Cl₆
Molecular Weight: 284.782
Melting Point (°C):
230.0 (Weast 1982–83)
228.83 (Lide 2003)
Boiling Point (°C):
322 (sublime, Weast 1982–83)
325 (Lide 2003)
Density (g/cm³):
1.5691 (23.6°C, Weast 1982–83; Horvath 1982)
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 Fusion, ΔH_{fus} (kJ/mol):
28.744 (Tsonopoulos & Prausnitz 1971)
22.40 (Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57.32 (Tsonopoulos & Prausnitz 1971)
44.77 (Miller et al. 1984)
Fugacity Ratio (assuming ΔS_{fusion} = 56 J/mol K), F: 0.010 (mp at 228.83°C)
0.0090 (25°C, Miller et al. 1985)
0.0075, 0.0094 (20°C, 25°C, Suntio et al. 1988)
Water Solubility (g/m³ or mg/L at 25°C):
0.005 (generator column-GC/ECD, Weil et al. 1974)
0.006 (shake flask-LSC/¹⁴C, Lu & Metcalf 1975)
0.110 (shake flask-nephelometry, Hollifield 1979)
0.005 (shake flask-UV, Yalkowsky et al. 1979)
0.0034 (calculated-K_{ope}, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
0.0035 (selected, Neely 1980)
0.036 (selected, Briggs 1981)
0.0039 (shake flask-GC, Könemann 1981)
0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)
0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)
0.005 (recommended, Horvath 1982)
0.0051 (Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.0066 (selected, Yoshida et al. 1983b)
0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0162 (calculated-UNIFAC activity coeff., Banerjee 1985)
0.005 (recommended, IUPAC 1985)
0.0146 (calculated-$K_{OW}$ and HPLC-RT, Chin et al. 1986)
0.006–0.2 (calculated-$K_{OW}$, Anliker & Moser 1987)
0.00537 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated):
0.00028 (Sears & Hopke 1949)
0.0015 (Callahan et al. 1979)
0.0026 (selected, OECD 1979)
0.00145 (20°C, Kiltzer et al. 1979)
0.0023 (gas saturation-GC, Farmer et al. 1980)
0.0013 (selected, Neely 1980; Suntio et al. 1988; Nash 1989)
0.000453; 0.000167 (Klein et al. 1981)
0.00046 (evaporation rate, Dobbs & Cull 1982)
0.00121 (extrapolated, Antoine eq., Gückel et al. 1982)
0.0006 (20°C, evaporation rate & gravimetric, Gückel et al. 1982)
0.0024 (20°C, Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.00147 (selected, Yoshida et al. 1983b)
0.303; 0.159; 0.121 (supercooled liquid $P_L$, selected; GC-RT, Bidleman 1984)
0.0031 (selected, Mackay et al. 1985)
0.00147, 0.187 (20°C, selected, solid, supercooled liquid, Bidleman & Foreman 1987)
0.245 (selected, Suntio et al. 1988; quoted, Bullschmier & Wittlinger 1991)
0.303, 0.127 (supercooled liquid, selected, Hinckley et al. 1990)
0.0023 (selected from Mackay et al. 1992, Mortimer & Connell 1995)
0.034; 0.141 (liquid $P_L$, GC-RT correlation; quoted lit., Donovan 1996)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
68.2 (20°C, Callahan et al. 1979)
5.07 (calculated-P/C, Mackay & Shiu 1981)
131.3 (batch stripping, Atlas et al. 1982)
68.9 (20°C, calculated, Mabey et al. 1982)
12.16 (calculated-P/C, Calamari et al. 1983)
62.0 (calculated-P/C, Yoshida et al. 1983b)
139 (calculated-P/C, Bobra et al. 1985)
48.6 (20°C, batch stripping, Oliver 1985)
133, 115.9 (observed, calculated-QSAR, Nirmalakhandan & Speece 1988)
7.12 (20°C, calculated-P/C, Suntio et al. 1988)
11.0 (calculated, Nash 1989)
139.0 (calculated-P/C, Fischer et al. 1991)

Octanol/Water Partition Coefficient, log $K_{OW}$:
6.18 (Neely et al. 1974; selected, McKim et al. 1985)
4.13 (radioisotope tracer-$^{14}C$, Lu & Metcalf 1975)
6.18 (selected, Callahan et al. 1979; Neuhauser et al. 1985)
4.13 (Hansch & Leo 1979)
5.0, 6.27 (shake flask-GC, HPLC-$k’$ correlation, Könemann et al. 1979; selected, Figueroa & Simmons 1991)
6.44 (calculated-f constant, Könemann et al. 1979; Könemann 1981; selected, Opperhuizen 1986)
5.23 (HPLC-RT correlation, Veith et al. 1979a; selected, Mackay 1982; Freitag et al. 1985)
6.18 (HPLC-RT, Veith et al. 1979b; quoted, Veith & Kosian 1982; Ryan et al. 1988; Saito et al. 1992)
5.23 (selected, Kenaga & Goring 1980; selected, Yoshida et al. 1983b)
5.44 (selected, Briggs 1981)
6.22 (HPLC-RT correlation, McDuffie 1981)
5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985; selected, Oliver & Niimi 1983; Oliver & Charlton 1984; Bobra et al. 1985; Hawker & Connell 1985; Oliver 1987a,b & c; Geyer et al. 1987; Suntio et al. 1988; Connell & Hawker 1988; Thomann 1989; Hawker 1990; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

5.66 (HPLC-RT correlation, Hammers et al. 1982)

5.40 (shake flask-GC, Watarai et al. 1982; quoted, Suntio et al. 1988)

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)

5.0, 5.19 (selected, calculated, Kaiser 1983; Kaiser et al. 1984)

5.89 (selected, Calamari et al. 1983)

6.42 (calculated-f const., Veith et al. 1983)

5.23, 4.61 (selected, calculated-molar refraction, Yoshida et al. 1983)


5.75; 5.70–5.79 (quoted lit.; HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)

5.20, 5.23, 5.44, 5.50, 5.55 (reported lit. values, Geyer et al. 1984)

5.47 (Sarna et al. 1984)

5.47, 6.86, 6.42 (selected, HPLC/MS, calculated-π const., Burkhard et al. 1985)

5.61 (selected, Mackay et al. 1985)

5.75 (selected OECD value, Brooke et al. 1986)

5.6, 5.9 (HPLC-RV correlation, Brooke et al. 1986)

6.51, 6.18 (selected, calculated-K_{ow} & HPLC-RT, Chin et al. 1986)

6.92 (HPLC-k' correlation, De Kock & Lord 1987)

5.64 (HPLC-k' correlation, Mailhot 1987)

5.45 (selected, Gobas et al. 1987, 1989; Travis & Arns 1988)

5.66 (correlated, Isnard & Lambert 1988, 1989)

5.47; 6.42, 6.55, 6.22, 5.34, 4.86, 4.75 (selected exptl.; calculated-π const., f const., HPLC-RT correlation, MW, MCI χ, TSA, Doucette & Andren 1988)

5.47; 5.37 (selected; calculated-V_{l} and solvatochromic parameters, Kamlet et al. 1988)

5.50 (shake flask-GC, Pereira et al. 1988)

5.31, 6.58 (selected, calculated-UNIFAC activity coeff., Banerjee & Howard 1988)

6.68 (calculated-f const., De Bruijn et al. 1989)

5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990; quoted, Bintein & Devillers 1994; Sijm et al. 1995)

5.44 (recommended, Sangster 1993)

5.73 (recommended, Hansch et al. 1995)

6.42 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

3.89 (rainbow trout, calculated-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. 1979)

5.46 (guppy, lipid basis, Könnemann & van Leeuwen 1980; selected, Chiou 1985)

4.27 (fish, Giam 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)

3.61, 2.45 (calculated from water solubility, K_{OC}, Kenaga 1980a)


3.91 (fish, correlated, Mackay 1982)

4.27, 3.89 (fathead minnow, rainbow trout, selected, Bysshe 1982)

4.60 (guppy, calculated-MCI χ, Koch 1983)

4.08–4.30 (rainbow trout, Oliver & Niimi 1983)

5.16–5.37 (rainbow trout, lipid basis, Oliver & Niimi 1983; selected, Chiou 1985)

4.31 (calculated-K_{ow}, Calamari et al. 1983)

3.93 (calculated-K_{ow}, Yoshida et al. 1983b)
Sorption Partition Coefficient, log $K_{OC}$:

- 3.59 (algae, fish, activated sludge, Klein et al. 1984)
- 4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
- 4.27 (fathead minnow, 25°C, calculated, Davies & Dobbs 1984; Anliker & Moser 1987)
- 4.34, 3.74 (green sunfish, rainbow trout, 15°C, calculated, Davies & Dobbs 1984)
- 4.39, 3.36, 4.54 (algae, fish, sludge, Klein et al. 1984)
- 4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
- 4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
- 3.05 (fish, selected, Hawker & Connell 1986)
- 2.62–2.97 (human fat, lipid basis, Geyer et al. 1987)
- 2.44–2.79 (human fat, 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)
- 4.19 (guppy, calculated, Gobas et al. 1987)
- 5.46 (guppy-lipid phase, calculated-$K_{ow}$, Gobas et al. 1987, 1989)
- 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)

- 4.41 (algae, calculated, Gobas et al. 1989)
- 3.53 (picea omorika, Reischl et al. 1989)
- 3.57 (fish, calculated, Figueroa & Simmons 1991)
- 4.37, 4.16 (rainbow trout, guppy, Saito et al. 1992)
- 4.27, 4.37 (fathead minnows, Saito et al. 1992)
- 4.25 (Chlorella pyrenoidosa, Sijm et al. 1995)
- 4.39, 3.18 (Chlorella fusca, Myriophyllum spicatum, Wang et al. 1996)

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

- 4.25 (shake flask-GC, soil-organic matter, Briggs 1981)
- 5.50 (Niagara River-organic matter, Oliver & Charlton 1984)
Sorption Partition Coefficient, log $K_P$:


5.11 (simulation of Oliver 1985, Brusseau & Rao 1989)

Half-Lives in the Environment:

- **Air**: degradation rate constant of 0.0144 h$^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991); 3753–37530 h, based on estimated photooxidation half-life (Atkinson 1987); 17000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

- **Surface Water**: 23256–50136 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 1.4–50 d estimated, 0.3–3 d for river water and 30–300 d for lakes, estimated from persistence (Zoeteman et al. 1980); 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

- **Ground Water**: 46512–100272 h, based on unacclimated aerobic biodegradation half-life (Beck & Hansen 1974); 30–300 d, estimated from persistence (Zoeteman et al. 1980).

- **Soil**: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen, 1974); > 50 d (Ryan et al. 1988).

- **Sediment**: 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

- **Biota**: half-life in rainbow trout, > 224 d (Niimi & Cho 1980); in subadult rainbow trout-calculated to be 210 d at 4°C, 80 d at 12°C and 70 d at 18°C (Niimi & Palazzo 1985); in worms at 8°C, 27 d (Oliver 1987a); picea omorika, 30 d (Reischl et al. 1989); 163 h, clearance from fish (Neely 1980).

Environmental Fate Rate Constants, $k$, or Half Lives, $t_{1/2}$:

**Volutilization/Evaporation**: $3.45 \times 10^{-10}$ mol/m$^2$·h (Gückel et al. 1982).

**Photolysis**:

- Oxidation: rate constant in air, $1.44 \times 10^{-2}$ h$^{-1}$ (Brown et al. 1975; selected, Mackay et al. 1985); photooxidation half-life in air: 3753–37530 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987).

**Hydrolysis**: not expected to be important, based on $k_h = 0$, observed after 13 d at pH 3, 7, 11 and 85°C (Ellington et al. 1987).

**Biodegradation**: aqueous aerobic biodegradation half-life: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974); anaerobic aqueous biodegradation half-life: 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974) and degradation rate constant in soil, $1.9 \times 10^{-5}$ h$^{-1}$ (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).

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

- $k_1$: 18.76 h$^{-1}$ (trout muscle, Neely et al. 1974)
- $k_2$: 0.00238 h$^{-1}$ (trout muscle, Neely et al. 1974)
- $k_1$: 10000 d$^{-1}$ (guppy, Könemann & van Leeuwen 1980)
- $k_1$: 22.5 h$^{-1}$ (guppy, selected, Hawker & Connell 1985)
- $k_1$: 18.8 h$^{-1}$ (trout, selected, Hawker & Connell 1985)
- $k_1$: 540.0 d$^{-1}$ (fish, selected, Opperhuizen 1986)
- $k_2$: 0.00510, 0.00818, 0.00640, 0.0047 d$^{-1}$ (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)
- $1/k_2$: 420 h (trout, selected, Hawker & Connell 1985)
- $\log k_1$: 2.73 d$^{-1}$ (fish, selected, Connell & Hawker 1988)
- $\log k_2$: 2.65 d$^{-1}$ (fish, selected, Connell & Hawker 1988)
- $\log 1/k_2$: 1.24 d$^{-1}$ (fish, calculated-$K_{OW}$, Thomann 1989)
- $k_1$: 0.049 h$^{-1}$ (uptake of mayfly-sediment model II, Gobas et al. 1989b)
- $k_2$: 0.023 h$^{-1}$ (depuration of mayfly-sediment model II, Gobas et al. 1989b)
- $k_1$: 10489 h$^{-1}$ (Chlorella fusca, Wang et al. 1996)
- $k_2$: 0.424 h$^{-1}$ (Chlorella fusca, Wang et al. 1996)
k₁: 6.558 h⁻¹ (Myriophyllum spicatum, Wang et al. 1996)
k₂: 0.00429 h⁻¹ (Myriophyllum spicatum, Wang et al. 1996)

Sediment Exchange Rate Constant:
0.026–1.2 d⁻¹ (natural sediment, Karickhoff & Morris 1985).

Sediment Burial Rate Constant:
4.6 × 10⁻⁶ h⁻¹ (Di Toro et al. 1981; selected, Mackay et al. 1985)

Stratospheric Diffusion Rate Constant:
1.7 × 10⁻⁶ h⁻¹ (Mackay et al. 1985)
19.1.23 IMAZALIL

Common Name: Imazalil
Synonym: Bromazil, Deccozil, Enilconazole, Fecundal, Freshgard, Fungafior, Fungazil, R 23979
Chemical Name: 1-[(β-allyloxy-2,4-dichlorophenylethyl)imidazole; 1-[2-(2,4-dichlorophenyl)-2-(2-propenylxy)ethyl]-1H-imidazole
CAS Registry No: 35554-44-0
Uses: as fungicide for control of a wide range of fungal diseases on fruit, vegetables, and ornamentals; also used as a seed dressing, for control of diseases of cereal and cotton, etc.

Molecular Formula: C_{14}H_{14}Cl_{2}N_{2}O
Molecular Weight: 297.129
Melting Point (°C):
- 50.0 (Hartley & Kidd 1987; Milne 1995; Lide 2003)
Boiling Point (°C):
- 340 (Worthing & Hance 1991; Tomlin 1994)
- dec (Lide 2003)
Density (g/cm³ at 20°C):
- 1.348 (26°C, Tomlin 1994)
Molar Volume (cm³/mol):
- 318.8 (calculated-Le Bas method at normal boiling point)
- 239.1 (calculated-density)
Dissociation Constant pKₐ:
- 6.53 (Worthing & Hance 1991)
- 7.47 (pKₐ Tomlin 1994)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
- 96.53 (Rordorf 1989)
Enthalpy of Fusion, ΔHₕᵤₛ (kJ/mol):
- 29.1 (Rordorf 1989)
Entropy of Fusion, ΔSₕᵤₛ (J/mol K):
- 90 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔSₕᵤₛ = 56 J/mol K), F: 0.568 (mp at 50°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 1400 (20°C, Hartley & Kidd 1987; Milne 1995)
- 180 (pH 7.6, Worthing & Hance 1991; Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
- 9.30 × 10⁻⁶ (20°C, Hartley & Kidd 1987)
- 1.60 × 10⁻⁴, 8.0 × 10⁻³, 0.230, 4.20, 53.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
-log (Pᵥ/Pₐ) = 18.21 – 6562.5/(T/K); measured range 53–129°C (solid, gas saturation-GC, Rordorf 1989)
-log (Pᵥ/Pₐ) = 13.52 – 5042.4/(T/K); measured range 53.6–129°C (liquid, gas saturation-GC, Rordorf 1989)
- 1.60 × 10⁻⁴ (20°C, Worthing & Hance 1991)
- 1.58 × 10⁻⁴ (20°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
  1.97 × 10⁻⁶ (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
  3.82 (Worthing & Hance 1991; Milne 1995)
  3.82 (pH 9.2, Tomlin 1994)
  3.82 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
  4.57 (calculated-S as per Kenaga 1980, this work)
  2.70 (calculated-$K_{\text{OW}}$ as per Kenaga 1980, this work)

Sorption Partition Coefficient, log $K_{\text{OC}}$:
  2.26 (clay loam, Worthing & Hance 1991; Tomlin 1994)
  2.32 (sandy loam, Worthing & Hance 1991; Tomlin 1994)
  1.83 (sandy soil, Worthing & Hance 1991; Tomlin 1994)
  3.73 (soil, calculated-MCI $'\chi'$, Sabljic et al. 1995)
  3.73; 3.52 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:
  Volatilization:
  Photolysis: stable to light under normal storage conditions (Tomlin 1994).
  Oxidation:
  Hydrolysis: very stable to hydrolysis in dilute acids and alkalis at room temperature (Tomlin 1994).
  Biodegradation:
  Biotransformation:
  Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
  Soil: $t_\frac{1}{2} = 30$–170 d (Tomlin 1994);
  field $t_\frac{1}{2} = 150$ d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
### 19.1.24 MANCOZEB

**Common Name:** Mancozeb  
**Synonym:** dithane ultra, Dithane M45, Dithane SPC, Fore, Manzate, Manseb, Maezin, Nemispor, Penncozeb, Vondozeb, Zimanat, zine manganese ethylenebis[dithiocarbamate]  
**Chemical Name:** manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt  
**CAS Registry No:** 8018-01-7

**Uses:** fungicide  
**Molecular Formula:** \((C_4H_6MnN_2S_4)_x(Zn)_y\)  
**Molecular Weight:**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>192–194 (dec., Hartley &amp; Kidd 1987; Montgomery 1993; Milne 1995)</td>
</tr>
<tr>
<td></td>
<td>192–204 (dec., Tomlin 1994)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>192–204 (dec., Tomlin 1994)</td>
</tr>
<tr>
<td>Density (g/cm^3) at 20°C</td>
<td>6–20 (Montgomery 1993)</td>
</tr>
<tr>
<td>Molar Volume (cm^3/mol)</td>
<td>6–20 (Tomlin 1994)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, (\Delta H_{\text{fus}}) (kJ/mol)</td>
<td>6.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)</td>
</tr>
<tr>
<td>Entropy of Fusion, (\Delta S_{\text{fus}}) (J/mol K)</td>
<td></td>
</tr>
</tbody>
</table>

**Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):**  
- insoluble (Spencer 1982; Hartley & Kidd 1987; Milne 1995)  
- 6–20 (Montgomery 1993)  
- 6–20 (Tomlin 1994)  

**Vapor Pressure (Pa at 25°C):**  
- negligible (Hartley & Kidd 1987; Tomlin 1994)  
- 0 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

**Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):**

**Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):**

- 3.12–3.70 (Montgomery 1993)

**Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):**

**Bioconcentration Factor, log \(B\text{CF}\):**

**Sorption Partition Coefficient, log \(K_{\text{oc}}\):**

- 2.93–3.21 (soil, calculated, Montgomery 1993)  
- > 3.30 (soil, Wauchope et al. 1992; Hornsby et al. 1996)  
- > 3.30 (soil, Tomlin 1994)

**Environmental Fate Rate Constants, or Half-Lives:**  
**Hydrolysis:** unstable in acidic media (Hartley & Kidd 1987); \(t_{1/2} = 20\) d at pH 5, \(t_{1/2} = 17\) h at pH 7, \(t_{1/2} = 34\) h at pH 9 (Montgomery 1993; Tomlin 1994).

**Half-Lives in the Environment:**  
- Soil: field \(t_{1/2} = 70\) d (Wauchope et al. 1992; Hornsby et al. 1996);  
- \(t_{1/2} \sim 6–15\) d (Tomlin 1994).
19.1.25 MANEB

![Chemical structure of Maneb]

Common Name: Maneb
Synonym: MEB, Dithane, Bravo
Chemical Name: manganese ethylenebis(dithiocarbamate)
CAS Registry No: 12427-38-2
Uses: fungicide
Molecular Formula: \((C_4H_6MnN_2S_4)_x\)
Molecular Weight: \((265.302)_x\)
Melting Point (°C): 200 (dec, Lide 2003)
Boiling Point (°C): 1.92 (Spencer 1982; Worthing & Walker 1983; Tomlin 1994)
Density (g/cm³ at 20°C): 1.92 (Spencer 1982; Worthing & Walker 1983; Tomlin 1994)
Molar Volume (cm³/mol): dissociation constant \(p_K_a\);
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):
- slightly soluble (Spencer 1982)
- slight, 200, 6 (quoted, Wauchope et al. 1992)
- 6.0 (20–25°C, estimated and selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

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, \(\log BCF\):
- 2.40 (activated sludge, Freitag et al. 1983)
- 2.40, 2.26, < 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

Sorption Partition Coefficient, \(\log K_{\text{OC}}\):
- > 3.30 (soil, estimated, Wauchope et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis: rapidly hydrolyzed in acidic media (Hartley & Kidd 1987);
  \(t_{1/2} < 24\) h at pH 5.7 or 9 (Tomlin 1994).
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (\(k_u\)) and Elimination (\(k_e\)) Rate Constants:
Half-Lives in the Environment:

Air: $t_{1/2} = 7\text{–}14\text{ d}$, green house experiment in microagroecosystem chamber (Nash & Beall 1980).

Surface water: rapidly hydrolyzed in acidic media (Hartley & Kidd 1987).

Groundwater:

Sediment:
Soil: $t_{1/2} = 36\text{ d}$ in soil (sandy loam with pH 6.7),
  green house experiment in microagroecosystem chamber (Nash & Beall 1980);
  $t_{1/2} \sim 25\text{ d}$ in loamy sand in dark, aerobic conditions (Tomlin 1994);
  field $t_{1/2} \sim 70\text{ d}$ (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: $t_{1/2} = 6.4\text{ d}$ for beans, $t_{1/2} = 7.4\text{ d}$ for tomatoes (Nash & Beall 1980);
  $t_{1/2} = 14\text{ d}$ on tomato leaves, green house experiment in microagroecosystem chamber (Nash & Beall 1980);
  $t_{1/2} = 10\text{ d}$ for tomato fruit, $t_{1/2} = 4.5\text{ d}$ for tomato leaves in the field, $t_{1/2} = 3\text{ d}$ for tomatoes and soybean leaves
  in microagroecosystem (Nash 1983).
19.1.26 Metalaxyl

Common Name: Metalaxyl
Synonym: Apron, CGA 48988, Ridomil, Subdue
Chemical Name: methyl N-(2-methoxyacetyl)-N-(2,6-xylyl)-DL-alaninate; methyl-N-(2,6-dimethylphenyl)-N-(methoxyacetyl)-DL-alaninate
CAS Registry No: 57837-19-1
Uses: fungicide to control of foliar and soil-borne diseases caused by *Peronosporates* on a wide range of crops; also used to treat seeds, etc.
Molecular Formula: \( \text{C}_{15}\text{H}_{21}\text{NO}_{4} \)
Molecular Weight: 279.333
Melting Point (°C):
71
(Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.21
(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
Molar Volume (cm³/mol):
328.2
(calculated-Le Bas method at normal boiling point)
230.9
(calculated-density)
Dissociation Constant \( \text{pK}_a \): << 0
(Tomlin 1994)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
89.73
(Rordorf 1989)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
27.4
(Rordorf 1989)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
79
(Rordorf 1989)
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \)), \( F \): 0.354 (mp at 71°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
7100
(quoted, Burkhard & Guth 1981)
7000
(shake flask-HPLC, Ellgehausen et al. 1981)
7100
7000
(quoted-Yalkowsky & Dannerfelser 1994, Pinsuwan et al. 1995)
8400
8400
(selected, Lohninger 1994)
8400
(22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.93 × 10⁻⁴
(20°C, volatilization rate, Burkhard & Guth 1981)
2.93 × 10⁻⁴
(20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
7.50 × 10⁻⁴, 2.90 × 10⁻², 0.67, 10.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
\[ \log (P_v/P_a) = 17.423 - 4687.6/(T/K); \text{measured range 32.7–69.7°C (solid, gas saturation-GC, Rordorf 1989)} \]
\[ \log (P_v/P_a) = 13.243 - 4687.6/(T/K); \text{measured range 72.3–130°C (liquid, gas saturation-GC, Rordorf 1989)} \]
7.5 × 10⁻⁴
2.93 × 10⁻⁴
(20°C, Montgomery 1993)
7.5 × 10⁻⁴
(Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):
1.155
(20°C, evaporation rate, Burkhard & Guth 1981)
2.48 × 10⁻⁵
(calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 1.65 (shake flask, Ellgehausen et al. 1980, 1981)
- 1.53 (shake flask, log P Database, Hansch & Leo 1987)
- 1.60 (shake flask at pH 7, Stevens et al. 1988)
- 1.70 (shake flask at pH 7, Baker et al. 1992)
- 1.59 (recommended value, Sangster 1993)
- 1.75 (Tomlin 1994)
- 1.693 (calculated-f const., Pinsuwan et al. 1995)
- 1.65 (recommended, Hansch et al. 1995)
- 1.40 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 0.03 ($Daphnia magna$, wet wt. basis, Ellgehausen et al. 1980)

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

- 1.59 (av. of 3 soils, Sharom & Edgington 1982)
- 2.26 (av. of 7 soils, Carris 1983)
- 3.22 (av. of 12 soils, calculated-linearized Freundlich Isotherm, Sukop & Cogger 1992)
- 1.53–1.84 (soil, estimated-chemical structure, Lohninger 1994)
- 1.70 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.57; 2.05 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

- Volatilization: $k$(calc) = 0.71 ng cm$^{-2}$ h$^{-1}$ and $k$(measured) = 0.35 ng cm$^{-2}$ h$^{-1}$ from moist soils at 20°C (Burkhard & Guth 1981).
- Photolysis: irradiated by UV at 290 nm in the presence of hydrogen peroxide and titanium dioxide, respectively, in aqueous solution resulted in 29% and 84% transformation in 2.5 h (Moza et al. 1994).
- Oxidation:
- Hydrolysis: stable in neutral and acidic media at room temp., calculated $t_\frac{1}{2}$ > 200 d at 20°C and pH 1, $t_\frac{1}{2}$ = 115 d at pH 9 and $t_\frac{1}{2}$ = 12 d at pH 10 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Biodegradation:

- degradation rate constant $k$ = 0.0081 h$^{-1}$ with $t_\frac{1}{2}$ = 85.5 h in sewage sludge and $k$ = 0.0217 d$^{-1}$ with $t_\frac{1}{2}$ = 31.9 d in garden soil (Müller & Buser 1995).
- rate constant $k$ = 0.060 d$^{-1}$ for R-metalaxyl (fungicidally active) in soil expt incubated with rac-metalaxyl,
- $k$ = 0.080 d$^{-1}$ in soil expt incubated with R-metalaxyl; rate constant $k$ = 0.015 d$^{-1}$ for S-metalaxyl (fungicidally inactive) in soil expt incubated with rac-metalaxyl, $k$ = 0.010/0.12 d$^{-1}$ for in soil expt incubated with S-metalaxyl (Buser et al. 2002);
- degradation rate constants for formulated racemic metalaxyl were found to be 0.039 d$^{-1}$ with $t_\frac{1}{2}$ = 18 d for German soil, $k$ = 0.018 d$^{-1}$ with $t_\frac{1}{2}$ = 38 d for Cameroonian soil; for unformulated racemic metalaxyl rate constants were: $k$ = 0.039 d$^{-1}$ with $t_\frac{1}{2}$ = 18 d for German soil, $k$ = 0.019 d$^{-1}$ with $t_\frac{1}{2}$ = 17 d form Cameroonian soil; and for formulated R-metalaxyl rate constants were: $k$ = 0.041 d$^{-1}$ with $t_\frac{1}{2}$ = 17 d for German soil, $k$ = 0.018 d$^{-1}$ with $t_\frac{1}{2}$ = 38 d from Cameroonian soil. For soil incubated with metalaxyl enantiomers, R-metalaxyl degraded faster ($k$ = 0.064 d$^{-1}$) than S-metalaxyl ($k$ = 0.033 d$^{-1}$) in German soil when spiked with formulated racemic metalaxyl, while S-metalaxyl degraded faster ($k$ = 0.026 d$^{-1}$) than R-metalaxyl ($k$ = 0.014 d$^{-1}$) in Cameroonian soil when spiked with formulated racemic retalaxyl (Monkiedje et al. 2003).

Biotransformation:

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

Half-Lives in the Environment:

- Soil: degradation $t_\frac{1}{2}$ = 39.5 d in garden soil (Müller & Buser 1995);
- field $t_\frac{1}{2}$ = 70 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
- residual activity in soil is about 70–90 d (Tomlin 1994);
- degradation $t_\frac{1}{2}$ = 17–38 d of the racemic mixture and enantiomers of metalaxyl in controlled incubation experiments in typical soils from Germany and Cameroon. (Monkiedje et al. 2003).
19.1.27 NITRACYL

Common Name: Nitrapyrin
Synonym: N-Serve
Chemical Name: 2-chloro-6-(trichloromethyl)pyridine
CAS Registry No: 1929-82-4
Uses: bactericide
Molecular Formula: C₆H₃Cl₄N
Molecular Weight: 230.907
Melting Point (°C):
63 (Lide 2003)
Boiling Point (°C):
136–137.5/11 mmHg (Tomlin 1994)
Density (g/cm³ at 25°C):
1.744 (Montgomery 1993)
1.579 (Tomlin 1994)
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
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: 0.424 (mp at 63°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
40 (quoted, Briggs 1981)
92; 54 (generator column-RI; HPLC-RT correlation, Swann et al. 1983)
Vapor Pressure (Pa at 25°C or as indicated):
0.37 (23°C, Spencer 1982; Worthing & Walker 1983, 1987)
0.373 (20°C, Montgomery 1993)
0.373 (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)
Henry's Law Constant (Pa·m³/mol at 25°C):
216 (calculated-P/C, Montgomery 1993)
Octanol/Water Partition Coefficient, log K_{ow}:
3.02 (shake flask-UV, Briggs 1981)
3.02–3.41 (Montgomery 1993)
3.325 (Tomlin 1994)
3.41 (recommended, Hansch et al. 1995)
3.41 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
1.87, 1.36 (calcd-solubility, K_{ow}, Kenaga 1980b)
Sorption Partition Coefficient, log K_{oc}:
1.93–2.42; 2.19 (quoted: 10 soils range; mean, Briggs 1981)
2.0 (Cottenham soil, shake flask-GC, 20°C, Briggs 1981)
2.76 (calculated, Kenaga 1980b)
2.66 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.64, 2.68, 2.66; 2.66 (Commeroe soil, Tracy soil, Catlin soil; mean, HPLC-RT, Swann et al. 1981; quoted, McCall et al. 1981)
2.24–2.76 (quoted literature range, Wauchope et al. 1992)
2.76 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
2.62–2.68 (soil, Montgomery 1993)
2.40–3.96 (soil, Tomlin 1994)
2.62 (soil, calculated-MCI ‘χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis: water photolysis t½ = 2 h (Tomlin 1994).
Oxidation:
Hydrolysis: hydrolysis t½ = 2 d at pH 7 (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: hydrolysis t½ = 2 d at pH 7, water photolysis t½ = 2 h (Tomlin 1994).
Groundwater:
Sediment:
Soil: field t½ = 10 d (Wauchope et al. 1992; Hornsby et al. 1992);
aerobic soil metabolism t½ = 6.42 d, anaerobic metabolism t½ ~ 2.5 h (Tomlin 1994).
Biota:
19.1.28 **Oxycarboxin**

![Oxycarboxin structure](image)

Common Name: Oxycarboxin  
Synonym: DCMOD, Oxycarboxine  
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathine-3-carboxanilide 4,4-dioxide; 5,6-dihydro-2-methyl-N-phenyl-1,4-oxathin-3-carboxamide 4,4-dioxide  
CAS Registry No: 5259-88-1  
Uses: as fungicide for control of rust diseases on ornamentals, cereals, and nursery trees, etc.  
Molecular Formula: C_{12}H_{13}NO_{4}S  
Molecular Weight: 267.301  
Melting Point (°C):  
129 (Lide 2003)  
Boiling Point (°C):  
Density (g/cm³ at 20°C): 1.14 (Tomlin 1994)  
Molar Volume (cm³/mol):  
261.4 (calculated-Le Bas method at normal boiling point)  
234.5 (calculated-density)  
Dissociation Constant pKₐ:  
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: 0.054 (mp at 129°C)  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
1000 (Martin & Worthing 1977; quoted, Kenaga 1980)  
1000 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
1000 (selected, Lohninger 1994)  
Vapor Pressure (Pa at 25°C or as indicated):  
0.0010 (20°C, Hartley & Kidd 1987)  
< 133 (20°C, Worthing & Hance 1991)  
5.60 × 10⁻⁶ (Tomlin 1994)  
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):  
3.56 × 10⁻⁴ (20–25°C, calculated-P/C, this work)  
Octanol/Water Partition Coefficient, log K_{OW}:  
0.74 (shake flask-UV, Mathre 1971)  
0.74 (recommended, Sangster 1993)  
0.772 (Tomlin 1994)  
0.740 (selected, Hansch et al. 1995)  
1.13 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)  
Bioconcentration Factor, log BCF:  
1.11 (calculated-S, Kenaga 1980)  
Sorption Partition Coefficient, log K_{OC}:  
1.99 (calculated-S, Kenaga 1980)
1.98  (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.98  (selected, Lohninger 1994)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Hydrolysis: $t_{1/2} = 44$ d at pH 6, 25°C (Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{1/2} = 2.5$–8 wk in sandy loam by aerobic soil metabolism (Tomlin 1994);
field $t_{1/2} = 20$ d (Wauchope et al. 1992; Hornsby et al. 1996).
19.1.29 **Penconazole**

Common Name: Penconazole

Synonym: Award, CGA 71818, Topas, Topaz, Topaze

Chemical Name: 1-(2,4-dichloro-β-propylphenylethyl)-1H-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)pentyl]-1H-1,2,4-triazole

CAS Registry No: 66246-88-6

Uses: as fungicide for control of pathogenic Ascomycetes, Basidiomycetes and Deuteromycetes (especially powdery mildews) on vines, cucurbits, pome fruit, ornamentals and vegetables.

Molecular Formula: C\textsubscript{13}H\textsubscript{15}Cl\textsubscript{2}N\textsubscript{3}

Molecular Weight: 284.184

Melting Point (°C):
- 60.0 (Hartley & Kidd 1987; Worthing & Hance 1991)
- 62.1 (Rordorf 1989)
- 57.6–60.3 (Tomlin 1994)

Boiling Point (°C):

Density (g/cm\textsuperscript{3} at 20°C): 1.30 (Tomlin 1994)

Molar Volume (cm\textsuperscript{3}/mol):
- 312.3 (calculated-Le Bas method at normal boiling point)
- 218.6 (calculated-density)

Dissociation Constant pK\textsubscript{a}:
- 1.51 (Tomlin 1994)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 91.45 (Rordorf 1989)

Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
- 27.1 (Rordorf 1989)

Entropy of Fusion, $\Delta S_{ fus}$ (J/mol K):
- 81 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{ fus} = 56$ J/mol K), F: 0.454 (mp at 60°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
- 70 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
- 73 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.00021 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- $3.70 \times 10^{-4}$, $1.30 \times 10^{-2}$, 0.28, 4.0, 41.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P\textsubscript{v}/Pa) = 16.671 − 5995.1/(T/K); measured range 36.6–58.3°C (solid, gas saturation-GC, Rordorf 1989)

log (P\textsubscript{v}/Pa) = 13.088 − 4777.0/(T/K); measured range 60.9–129°C (liquid, gas saturation-GC, Rordorf 1989)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C or as indicated):
- 0.00082 (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 3.40 (shake flask-HPLC, Bateman et al. 1990)
- 3.20 (shake flask-HPLC, Chamberlain et al. 1991)
Fungicides

3.72 (pH 5.7, Tomlin 1994)
3.40, 3.20 (Sangster 1993)
3.40, 3.50 (Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.75 (20°C, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
2.62 (20°C, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Hydrolysis: stable to hydrolysis pH 1–13, and to temperature up to 350°C (Tomlin 1994).

Half-Lives in the Environment:
Soil: half-life is several months (Tomlin 1994).
19.1.30 Procymidone

Common Name: Procymidone
Synonym: S-7131, Sialex, Sumiboto, Sumilex, Sumiselex
Chemical Name: \( \text{N-(3,5-dichlorophenyl)-1,2-dimethylcyclopropane-1,2-dicarboximide; } 3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3,1,0]hexane-2,4-dione \)
CAS Registry No: 32809-16-8
Uses: as fungicide for control of Botrytis, Sclerotinia, Monilia, and Helminthosporium spp. on fruit, vines, vegetables, cereals and ornamentals, etc.
Molecular Formula: \( \text{C}_{13}\text{H}_{11}\text{Cl}_{2}\text{NO}_{2} \)
Molecular Weight: 284.138
Melting Point (°C): 166 (Lide 2003)
Boiling Point (°C):
Density (g/cm\(^3\) at 20°C):
\( 1.452 \) (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm\(^3\)/mol):
\( 225.9 \) (calculated-Le Bas method at normal boiling point)
\( 195.7 \) (calculated-density)
Dissociation Constant \( \text{pK}_a \):
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 \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \)), \( F \): 0.0414 (mp at 166°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
\( 4.50 \) (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
\( 0.018 \) (Hartley & Kidd 1987)
\( 0.011 \) (20°C, Worthing & Hance 1991)
\( 0.018, 0.0105 \) (20, 25°C, Tomlin 1994)
\( 0.0187 \) (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C or as indicated):
\( 1.181 \) (20–25°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):
\( 3.0 \) (selected, Hansch et al. 1995)
Bioconcentration Factor, \( \log BCF \):
\( 2.42 \) (calculated-S as per Kenaga 1980, this work)
Sorption Partition Coefficient, \( \log K_{\text{oc}} \):
\( 3.18 \) (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
\( 3.28 \) (soil, calculated-S as per Kenaga 1980, this work)
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Photolysis: when irradiation with UV light, λ ≥ 290 nm, for procymidone solution (2 ppm): 9% and 11% photo-degraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; rapid degradation with t½ = 3 min in the presence of TiO₂ (20 ppm), but degraded slowly as 9% transformation in 2 h with Fe₂O₃ (100 ppm). (Hustert & Moza 1997)

Half-Lives in the Environment:
Air:
Surface water: photodegradation of procymidone solution (2 ppm), t½ = 3 min in the presence of TiO₂ (20 ppm) when irradiated with UV light (Hustert & Moza 1997)

Groundwater:

Sediment:
Soil: persists for ca. 4–12 weeks (Hartley & Kidd 1987; Tomlin 1994);
field t½ = 7 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:
19.1.31 Propargite

Common Name: Propargite
Synonym: Comite, Omite
Chemical Name: 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite
CAS Registry No: 2312-35-8
Uses: acaricide
Molecular Formula: C_{16}H_{26}O_{4}S
Molecular Weight: 360.472
Melting Point (°C): dark brown liquid (Hartley & Kidd 1987)
Boiling Point (°C):
Density (g/cm³ at 25°C):
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
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):
practically insoluble in water (Worthing & Walker 1983, 1987)
0.5 (20°C, Hartley & Kidd 1987)
0.50 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.5 (20–25°C, Majewski & Capel 1995)
Vapor Pressure (Pa at 25°C or as indicated):
0.4 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.4 (20–25°C, quoted, Majewski & Capel 1995)
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}:
3.60 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Soil: field t_{1/2} = 40 and 56 d, the recommended t_{1/2} = 56 d (Wauchope et al. 1992; Hornsby et al. 1996).
**19.1.32 P R O P I C O N A Z O L E**

![Chemical Structure](image)

**Common Name:** Propiconazole  
**Synonym:** Alamo, Banner, CGA 64250, Desmel, Orbit, Practis, Radar, Spire, Tilt  
**Chemical Name:** (±)-1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole  
**CAS Registry No:** 60207-90-1

**Uses:** as fungicide for control of mildews, rusts on cereals, ornamentals, fruits and other crops; and also used for other diseases of turf and grass seed crops, etc.

**Molecular Formula:** C₁₅H₁₇Cl₂N₃O₂  
**Molecular Weight:** 342.221

**Melting Point (°C):** liquid  
**Boiling Point (°C):**  
180 (at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

**Density (g/cm³ at 20°C):**  
1.27 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)  
1.29 (20°C, Tomlin 1994)

**Molar Volume (cm³/mol):**  
358.6 (calculated-Le Bas method at normal boiling point)  
267.3 (calculated-density)

**Dissociation Constant pKₐ:**  
1.09 (Tomlin 1994)

**Enthalpy of Vaporization, ΔHᵥ (kJ/mol):**  
106.8 (Rordorf 1989)

**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:** 1.0

**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
110 (20°C, Hartley & Kidd; Worthing & Hance 1991; Milne 1995)  
100 (20°C, Tomlin 1994)  
110 (selected, Lohninger 1994)  
110 (20°C, quoted, Siebers et al. 1994)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**  
0.00013 (20°C, Hartley & Kidd 1987)  
5.60 × 10⁻⁵, 1.60 × 10⁻³, 0.027, 0.32, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
log (P/Pₐ) = 14.468 – 5581.2/(T/K); measured range 32.5–124°C (liquid, gas saturation-GC, Rordorf 1989)  
0.000133 (20°C, Worthing & Hance 1991)  
5.6 × 10⁻⁵ (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)  
5.6 × 10⁻⁵ (Tomlin 1994)

**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):**  
4.0 × 10⁻⁴ (20°C, calculated-P/C, Siebers et al. 1994)  
0.00017 (20–25°C, calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 3.50 (Bateman et al. 1990; quoted, Sangster 1993)
- 3.72 (Siebers et al. 1994)
- 3.72 (pH 6.6, Tomlin 1994)
- 3.50 (selected, Hansch et al. 1995)
- 3.50 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
- 2.81 (soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.52 (soil, calculated-S as per Kenaga 1980, this work)
- 2.81 (selected, Lohninger 1994)
- 3.39 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
  - Hydrolysis: no significant hydrolysis (Tomlin 1994).

Half-Lives in the Environment:
  - Air:
    Surface water: $t_{1/2} = 25–85$ d in aerobic aquatic systems at 25°C (Tomlin 1994).
  - Groundwater:
  - Sediment:
    Soil: field $t_{1/2} = 110$ d (Wauchope et al. 1992; Hornsby et al. 1996);
    $t_{1/2} = 40–70$ d in aerobic soils at 25°C (Tomlin 1994).
  - Biota:
19.1.33 QUINOZENE

Common Name: Quintozene
Synonym: Avicol, Batrilex, Brassicol, Chinozan, earthcide, Fartox, Folosan, Fomac 2, Fungiclor, Kobutol, KOBU, KP 2, Marisan forte, Olpisan, PCNB, Pentagen, Phomasan, PKhNB, Quinosan, Quinocene, saniclor 30, Terraclor, Terrafun
Chemical Name: pentachloronitrobenzene
CAS Registry No: 82-68-8
Uses: as fungicide for seed and soil treatment, for control of Botrytis, Rhizoctonia, and Sclerotinia spp. on brassicas, vegetables, ornamentals and other crops, and Tilletia caries of wheat.

Molecular Formula: C_6Cl_5NO_2
Molecular Weight: 295.335
Melting Point (°C):
144 (Lide 2003)
Boiling Point (°C):
328 (dec, Lide 2003)
Density (g/cm³ at 20°C):
1.907 (21°C, Tomlin 1994)
Molar Volume (cm³/mol):
207.3 (calculated-Le Bas method at normal boiling point)
154.9 (calculated-density)
Dissociation Constant pKₐ:
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
77.3 (Rordorf 1989)
Enthalpy of Fusion, ΔH₉₉s (kJ/mol):
18 (Rordorf 1989)
Entropy of Fusion, ΔS₉₉s (J/mol K):
43 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS₉₉s = 56 J/mol K), F: 0.0680 (mp at 144°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
practically insoluble (Spencer 1982; Worthing & Hance 1991; Milne 1995)
0.55 (20–25°C, shake flask-GC, Kanazawa 1981)
0.44 (20°C, Hartley & Kidd 1987; Pait et al. 1992; Milne 1995)
0.40 (Davies & Lee 1987)
0.44 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.10 (selected, Lohninger 1994)
0.10 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0151 (Spencer 1982)
6.60 × 10⁻³ (20°C, Hartley & Kidd 1987)
8.40 × 10⁻³, 0.16, 1.90, 17.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pₐ) = 14.34 − 4893.9/(T/K); measured range 49.9−140°C (solid, gas saturation-GC, Rordorf 1989)
log (Pᵥ/Pₐ) = 12.234 − 4037.9/(T/K); measured range 150–196°C (liquid, gas saturation-GC, Rordorf 1989)
1.80 (Worthing & Hance 1991)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0127 (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):

- 0.3718 (known LWAPC of Kawamoto & Urano 1989, Meylan & Howard 1991)
- 0.4812 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)

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

- 4.22 (20°C, shake flask-GC, Kanazawa 1981)
- 5.21 (HPLC-RT correlation, McDuffie 1981)
- 5.00 (HPLC-RT correlation, Ohori & Ihashi 1987)
- 5.18 (HPLC-RT correlation, Kawamoto & Urano 1989)
- 4.77; 5.40 (shake flask-GC; calculated-fragment const., Niimi et al. 1989)
- 5.02 (RP-HPLC-RT correlation, Saito et al. 1993)
- 4.64 (recommended, Sangster 1993)
- 5.0–6.0 (Tomlin 1994)
- 4.22 (selected, Hansch et al. 1995)
- 4.89 (Pomona-database, Müller & Kördel 1996)
- 5.01 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 5.30 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.38 (topmouth gudgeon, Kanazawa 1981)
- 3.49, 3.65, 3.06 (algae, activated sludge, fish, Freitag et al. 1985)
- 2.23 (rainbow trout, Niimi et al. 1989)
- 2.91 (quoted, Pait et al. 1992)

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

- 4.30 (correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
- 4.30, 3.38 (soil, quoted exptl., calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
- 3.70 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 4.34 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
- 3.78, 3.47 (for adsorption: silt loam, sand, Tomlin 1994)
- 3.98, 3.52 (for desorption: silt loam, sand, Tomlin 1994)
- 4.30 (estimated-chemical structure, Lohninger 1994)
- 4.34; 3.38 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

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

Biodegradation: rate constant $k$(aerobic) = 0.16 d$^{-1}$ with $t_{1/2} = 4.3$ d at 20°C by aerobic activated sludge and $k$(anaerobic) = 0.16 d$^{-1}$ with $t_{1/2} = 4.3$ d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)

rate constant $k = 6.5$ d$^{-1}$ with $t_{1/2} = 0.11$ d (Corrigendum, Kawamoto & Urano 1991).

Half-Lives in the Environment:

Air:
Surface water: biodegradation $t_{1/2} = 4.3$ d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)

Groundwater:

Sediment:
Soil: $t_{1/2} \sim 4–10$ months (Hartley & Kidd 1987; Tomlin 1994), $t_{1/2} = 4$ d (Pait et al. 1992); field $t_{1/2} = 21$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:
### 19.1.34 Thiophanate-methyl

![Chemical Structure](image)

**Common Name:** Thiophanate-methyl  
**Synonym:** Cerobin, Enovit, Fumidor, Fungitox, Fungo, Fungus Fighter, Labilite, Mildothane, Neotosin, NF-44, Pelt 44, Seal 7 Heal, Sigma, Sipcaplant, Sipcasan, Topsisin M, Trevin  
**Chemical Name:** dimethyl 4,4′-(o-phenylene)bis(3-thioallophanate; dimethyl [1,2-phenylene-bis(monocarbonothioyl)]-biscarbamate  
**Uses:** fungicide/wound protectant  
**CAS Registry No:** 23564-05-8  
**Molecular Formula:** C₁₂H₁₄N₄O₄S₂  
**Molecular Weight:** 342.394  
**Melting Point (°C):** 172 (dec., Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³ at 20°C):**  
**Molar Volume (cm³/mol):** 344.0 (calculated-Le Bas method at normal boiling point)  
**Dissociation Constant pK_a:** 7.28 (Worthing & Hance 1991; Tomlin 1994)  
**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:** 0.0361 (mp at 172°C)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
3.50 (20°C, Hartley & Kidd 1987)  
26.6 (Worthing & Hance 1991)  
3.50 (selected, Lohninger 1994)  
26.6 (20°C, Milne 1995)  
**Vapor Pressure (Pa at 25°C or as indicated):**  
< 1.0 × 10⁻⁵ (20°C, Hartley & Kidd 1987)  
9.50 × 10⁻⁶ (Tomlin 1994)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):** 0.0013 (calculated-P/C, this work)  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
1.40 (Worthing & Hance 1991; Milne 1995)  
1.50 (Tomlin 1994)  
1.40 (selected, Hansch et al. 1995)  
1.86 (RP-HPLC-RT correlation, pH 3.5, Hu et al. 1997)
Bioconcentration Factor, log BCF:

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

- 0.079 (Worthing & Hance 1991)
- 3.26 (selected, Lohninger 1994)

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

- Hydrolysis: stable neutral, aqueous solution, $t_\frac{1}{2} = 24.5$ h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

- Soil: field $t_\frac{1}{2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996);
  persistence ca. 3–4 weeks (Tomlin 1994).
**Fungicides 4097**

**19.1.35 Thiram**

Common Name: Thiram
Chemical Name: tetramethylthiuram disulphide; bis(dimethylthiocarbamoyl) disulfide
CAS Registry No: 137-26-8
Uses: fungicide and also as seed disinfectant.
Molecular Formula: C₆H₁₂N₂S₄
Molecular Weight: 240.432
Melting Point (°C): 155.6 (Lide 2003)
Boiling Point (°C): 129 (20 mmHg, Howard 1991)
310–315 (15 mmHg, Montgomery 1993)
Density (g/cm³ at 20°C): 1.29 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
256.6 (calculated-Le Bas method at normal boiling point)
186.4 (calculated-density)
Dissociation Constant pKₐ:
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: 0.0523 (mp at 155.6°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
17.4 (22°C, Spencer 1973, 1982)
30 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
30 (Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
18 (room temp., Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
negligible (Hartley & Kidd 1987; Worthing & Hance 1991)
0.00133 (Halfon et al. 1996)
< 0.00133 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.307 (Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
< 0.008 (calculated-P/C, Lyman et al. 1982)
0.0107 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log Kₐₗₘ:\n1.73 (Tomlin 1994)
Bioconcentration Factor, log BCF:
1.96 (calculated-S, Kenaga 1980)
1.96 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
Sorption Partition Coefficient, log $K_{OC}$:

- 2.83 (calculated-S, Kenaga 1980)
- 2.83 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
- 2.82–3.39 (soil, Montgomery 1993)
- 2.83 (estimated-chemical structure, Lohninger 1994)

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

- Volatilization:
  - Photolysis:
    - Oxidation: assuming an ambient hydroxyl radical concn. of $8.0 \times 10^5$ mol/cm$^3$, the photooxidation reaction $t_\frac{1}{2} \approx 26.6$ d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).
    - Hydrolysis: $t_\frac{1}{2} = 5.3$ d was estimated based on exp. rate $k = 5.0 \times 10^{-3}$ h$^{-1}$ (Ellington et al. 1988; quoted, Howard 1991; Montgomery 1993);
      - $t_\frac{1}{2} = 128$ d at pH 4, $t_\frac{1}{2} = 18$ d at pH 7 and $t_\frac{1}{2} = 9$ h at pH 9 (Tomlin 1994).
  - Biodegradation:
  - Biotransformation:
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: assuming an ambient hydroxyl radical concn. of $8.0 \times 10^5$ mol/cm$^3$, the photooxidation reaction $t_\frac{1}{2} \approx 26.6$ d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).
- Surface water: calculated hydrolysis $t_\frac{1}{2} = 5.3$ d at pH 7 (Ellington et al. 1988);
  - hydrolysis $t_\frac{1}{2} = 128$ d, $t_\frac{1}{2} = 18$ d and $t_\frac{1}{2} = 9$ h at pH 4,7 and 9 (Tomlin 1994).
- Groundwater:
- Sediment:
- Soil: $t_\frac{1}{2} = 15$ d in soil (Halfon et al. 1996);
  - field $t_\frac{1}{2} = 15$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
  - degradation $t_\frac{1}{2} = 0.5$ d in sandy soil at pH 6.7 (Tomlin 1994).
- Biota:
19.1.36 TOLCLOFOS-METHYL

Common Name: Tolclofos-methyl
Synonym: Risolex, Rizolex, S-3349
Chemical Name: O-2,6-dichloro-p-tolyl O,O-dimethyl phosphorothioate; O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl phosphorothioate
CAS Registry No: 57018-04-9
Uses: as fungicide for control of soil-borne diseases caused by Rhizoctonia, Sclerotium and Typhula spp.; also used as a seed, bulb or tuber treatment, soil drench, foliar spray, or by soil incorporation.
Molecular Formula: C\textsubscript{9}H\textsubscript{11}Cl\textsubscript{2}O\textsubscript{3}PS
Molecular Weight: 301.127
Boiling Point (°C):
Dissociation Constant pK\textsubscript{a}:
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):
0.3–0.4 (23°C, Hartley & Kidd 1987)
0.3–0.4 (23°C, Worthing & Hance 1991)
1.10 (Tomlin 1994)
0.30 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Vapor Pressure (Pa at 25°C or as indicated):
0.057 (20°C, Hartley & Kidd 1987)
0.057 (20°C, Worthing & Hance 1991; Tomlin 1995)
0.0573 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.25 × 10\textsuperscript{–3}; 6.61 × 10\textsuperscript{–3}, 0.0234 (gradient GC method; estimation using modified Watson method: Sugden’s parachor, McGowan’s parachor, Tsuzuki 2000)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
57.5 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K\textsubscript{ow}:
4.56 (Worthing & Hance 1991; Tomlin 1994)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K\textsubscript{OC}:
3.30 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Photolysis: photodegradable with 8 h of sunlight: $t_{1/2} = 44$ d in water, $t_{1/2} = 15–28$ d in lake and river water, and $t_{1/2} < 2$ d on soil surface (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: photodegradable with 8 hours of sunlight in water with $t_{1/2} = 44$ d, $t_{1/2} = 15–28$ d in lake and river water, and $t_{1/2} < 2$ d on soil surface (Hartley & Kidd 1987);
Photodegradation $t_{1/2} = 44$ d in water, $t_{1/2} = 15–28$ d in lake (Tomlin 1994).

Groundwater:

Sediment:

Soil: $t_{1/2} < 2$ d from soil surface by photodegradation (Tomlin 1994);
field $t_{1/2} = 30$ d (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Biota:
**19.1.37 TOLYLFUANID**

![Chemical structure of Tolylfluanid](image)

Common Name: Tolylfuanid  
Synonym: Tolylfluanide

Chemical Name: \(N\)-dichlorofluoromethylthio-\(N\)'\(N\)'-dimethyl-\(N\)-\(p\)-tolylsulphamide; 1,1-dichloro-\(N\)-[(dimethylamino)sulfonyl]-1-fluoro-\(N\)-(4-methylphenyl)methane-sulfenamide

Uses: fungicide/acaricide; to control scab on apples and pears; *Botrytis* on strawberries, raspberries, blackberries, currants, grapes, ornamentals, etc.

CAS Registry No: 731-27-1

Molecular Formula: \(C_{10}H_{13}Cl_{2}FN_{2}O_{2}S_{2}\)

Molecular Weight: 347.257

Melting Point (°C):
- 95–97 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
- 96 (Tomlin 1994)

Boiling Point (°C): dec. on distillation (Tomlin 1994)

Density (g/cm² at 20°C): 1.52 (Tomlin 1994)

Molar Volume (cm³/mol):
- 326.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(pK_a\):

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), \(F\): 0.201 (mp at 96°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 4000 (Martin & Worthing 1977; quoted, Kenaga 1980)
- 4000 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)
- 0.90 (room temp., Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
- < 0.001 (20°C, Hartley & Kidd 1987)
- \(1.3 \times 10^{-5}\) (45°C, Worthing & Hance 1991)
- \(1.6 \times 10^{-5}\) (20°C, Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, \(\log K_{ow}\):
- 3.95 (20°C, Worthing & Hance 1991)
- 3.90 (Tomlin 1994)
- 3.95 (selected, Hansch et al. 1995)
- 4.36 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, \(\log BCF\):
- 0.778 (calculated, Kenaga 1980)

Sorption Partition Coefficient, \(\log K_{OC}\):
- 1.66 (soil, calculated-S, Kenaga 1980)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 12$ d at $22^\circ$C and pH 4, $t_{1/2} = 29$ h at pH 7 and $t_{1/2} < 10$ min at pH 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life of a few days (Tomlin 1994).
Fungicides

19.1.38 TRIADIMEFON

Common Name: Triadimefon
Synonym: Amiral, Bayleton, MEB 6447, Triadimefone
Chemical Name: 1-(4-chlorophenoxy)-3,3-dimethyl-1-((1H-1,2,4-triazol-1-yl)butanone; 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone
CAS Registry No: 43121-43-3
Uses: as fungicide for control of powdery mildews, rusts in cereals and Rhynchosporium in cereals and control of bunt, smuts, Typhula spp., seedling blight, leaf stripe, net blotch, and other cereal diseases when used for seed treatment, etc.
Molecular Formula: C_{14}H_{16}ClN_{3}O_{2}
Molecular Weight: 293.749
Melting Point (°C):
   82 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
   1.22 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm³/mol):
   321 (calculated-Le Bas method at normal boiling point)
   240.8 (calculated-density)
Dissociation Constant pKₐ:
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: 0.276 (mp at 82°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   260 (Martin & Worthing 1977)
   71.5 (selected, Lohninger 1994)
   64 (20°C, Tomlin 1994)
   69; 72 (calculated-group contribution fragmentation method; quoted exptl., Kühne et al. 1995)
Vapor Pressure (Pa at 25°C or as indicated):
   < 1.0 × 10⁻⁴ (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
   2.00 × 10⁻⁶ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
   2.00 × 10⁻⁵, 6.0 × 10⁻⁵ (20, 25°C, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
   1.80 (shake flask-UV at pH 5, Barak et al. 1983)
   3.26 (shake flask, Hansch & Leo 1987)
   2.77 (shake flask-LC, Patil et al. 1988)
   3.18 (Worthing & Hance 1991; Milne 1995)
   2.90 (shake flask at pH 7, Baker et al. 1992)
   3.26 (recommended, Sangster 1993)
   2.77 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:  
1.43 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K OC:  
2.41 (soil, calculated-S, Kenaga 1980)  
2.57 (HPLC-screening method, Kördel et al. 1993)  
2.48 (estimated-chemical structure, Lohninger 1994)  
2.48 (soil, Tomlin 1994)  
2.71 (soil, calculated-MCI χ, Sabljic et al. 1995)  
2.57; 3.72 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
2.71; 2.43 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t½:  
Hydrolysis: t½ > 1 yr at 22°C and pH 3, 6, and 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:  
**19.1.39 TRIFLUMIZOLE**

![Chemical Structure of Triflumizole](image)

**Common Name:** Triflumizole  
**Synonym:** NF-114, Triflumizol, Trifmine  
**Chemical Name:** (E)-4-chloro-α,α,α-trifluoro-N-(1-imidazol-1-yl-2-propoxyethylidene)-o-toluidine; 1-[1-[(4-chloro-2-(trifluoromethyl)phenyl)imino]-2-propoxyethyl]-1H-imidazole  
**CAS Registry No:** 68694-11-1  
**Uses:** as fungicide for control of powdery mildews in fruit, vines, and vegetables; scab and rust in apples and pears; also used as seed treatment for barley, etc.

**Molecular Formula:** C₁₅H₁₅ClF₃N₃O  
**Molecular Weight:** 345.574

**Melting Point (°C):**  

**Boiling Point (°C):**  

**Density (g/cm³ at 20°C):**  

**Molar Volume (cm³/mol):**  
359.5 (calculated-Le Bas method at normal boiling point)

**Dissociation Constant pKₐ:**  

**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:** 0.419 (mp at 63.5°C)

**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
1.25 × 10⁻³ (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)  

**Vapor Pressure (Pa at 25°C or as indicated):**  
1.40 × 10⁻⁶ (Worthing & Hance 1991)  
1.86 × 10⁻⁴ (Tomlin 1994)

**Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated):**  
4.07 × 10⁻⁸ (20–25°C, calculated-P/C, this work)

**Octanol/Water Partition Coefficient, log Kₐw:**  
1.40 (selected, Hansch et al. 1995)

**Sorption Partition Coefficient, log Kₐw:**  
3.03–3.22 (Tomlin 1994)  
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Photolysis: aqueous solutions degraded by sunlight with $t_{1/2} = 29$ h (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} = 14$ d on clay (Worthing & Hance 1991);
Common Name: Triforine
Synonym: Biiformyloholin, Cela W524, Compound W, Denarin, FMC, Funginex, Saprol, W 524
Chemical Name: 1,1′-piperazine-1,4-diyl-di-[N-(2,2,2-trichloroethyl)formamide]; 1,4-bis(2,2,2-trichloro-1-formamidoethyl)piperazine; N,N′-[1,4-piperazinediylyls(2,2,2-trichloro-ethylidene)]bisformamide
Uses: systemic fungicide to control powdery mildews on cereals, fruit, vines, hops, cucurbits, vegetables, and ornamentals, etc.; also used to suppress spider mite activity.
CAS Registry No: 26644-46-2
Molecular Formula: C_{10}H_{14}Cl_{6}N_{4}O_{2}
Molecular Weight: 434.962
Boiling Point (°C): Density (g/cm³ at 20°C): 1.554 (Tomlin 1994)
Molar Volume (cm³/mol):
389.2 (calculated-Le Bas method at normal boiling point)
279.9 (calculated-density)
Dissociation Constant pKₐ:
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: 0.053 (mp at 155°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
30 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991)
6.0 (rm. temp., Worthing & Hance 1991; Milne 1995)
30 (selected, Lohninger 1994)
9.0 (20°C, Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
2.6 × 10⁻⁵ (Hartley & Kidd 1987)
2.7 × 10⁻⁵ (Worthing & Hance 1991; Tomlin 1994)
2.7 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
2.20 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
2.30 (estimated-chemical structure, Lohninger 1994)
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Hydrolysis: t_{1/2} = 3.5 d at pH 5, 25°C in aqueous solutions (Tomlin 1994).
Half-Lives in the Environment:
Soil: t_{1/2} ~ 3 wk in soil (Hartley & Kidd 1987; Tomlin 1994);
## 19.1.41 Vinclozolin

**Common Name:** Vinclozolin  
**Synonym:** BAS 352F, Ronilan, V orlan  
**Chemical Name:** (RS)-3-(3,5-dichlorophenyl)-5-vinyl-1,3-oxazolidine-2,4-dione; 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione  
**CAS Registry No:** 50471-44-8

**Uses:** fungicide to control Botrytis/Sclerotinia spp. in vines, oilseed rape, vegetables, fruit, and ornamentals, etc.

**Molecular Formula:** C₁₂H₉Cl₂NO₃  
**Molecular Weight:** 286.110

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiling Point (°C)</td>
<td>131 (at 0.05 mmHg, Hartley &amp; Kidd 1987; Tomlin 1994; Milne 1995)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>1.51 (Worthing &amp; Hance 1991; Tomlin 1994; Milne 1995)</td>
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<tr>
<td>Molar Volume (cm³/mol)</td>
<td>266.3 (calculated-Le Bas method at normal boiling point, this work)</td>
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<td></td>
<td>189.5 (calculated-density, this work)</td>
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<tr>
<td>Dissociation Constant pKₐ</td>
<td></td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔHₘₚ (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ΔSₘₚ (J/mol K)</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F: 0.153 (mp at 108°C)</td>
<td></td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated):</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>(Martin &amp; Worthing 1977)</td>
</tr>
<tr>
<td>1000</td>
<td>(20°C, Hartley &amp; Kidd 1987)</td>
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<tr>
<td>Vapor Pressure (Pa at 25°C or as indicated):</td>
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</tr>
<tr>
<td>&lt; 0.010</td>
<td>(20°C, Hartley &amp; Kidd 1987)</td>
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<tr>
<td>1.6 × 10⁻⁵</td>
<td>(20°C, Worthing &amp; Hance 1991; Tomlin 1994)</td>
</tr>
<tr>
<td>1.6 × 10⁻⁵</td>
<td>(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)</td>
</tr>
<tr>
<td>1.3 × 10⁻⁴</td>
<td>(20°C, Siebers et al. 1994)</td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa⁻¹mol at 25°C or as indicated):</td>
<td></td>
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<tr>
<td>0.011</td>
<td>(20°C, quoted, Siebers et al. 1994)</td>
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<td>Octanol/Water Partition Coefficient, log Kₕₖw:</td>
<td></td>
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<td>3.00</td>
<td>(Stevens et al. 1988)</td>
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<tr>
<td>3.00</td>
<td>(pH 7, Worthing &amp; Hance 1991; Tomlin 1994; Milne 1995)</td>
</tr>
<tr>
<td>2.47</td>
<td>(shake flask-HPLC at pH 6, Nielsen et al. 1992)</td>
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<tr>
<td>3.00, 2.47</td>
<td>(Sangster 1993)</td>
</tr>
<tr>
<td>3.10</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>Bioconcentration Factor, log BCF:</td>
<td></td>
</tr>
<tr>
<td>1.26</td>
<td>(calculated, Kenaga 1980)</td>
</tr>
</tbody>
</table>
Fungicides

Sorption Partition Coefficient, log $K_{OC}$:
- 1.99 (soil, calculated-S, Kenaga 1980)
- 2.0–2.87 (soil, Tomlin 1994)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:
- **Volatilization:**
  - Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for vinclozolin aqueous solution (1 ppm): 10% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; irradiation of vinclozolin (2 ppm) in water with $t_\text{½} = 7$ min and 92 min in the presence of TiO$_2$ (20 ppm), and Fe$_2$O$_3$ (100 ppm), respectively. (Hustert & Moza 1997)
- **Oxidation:**
  - Hydrolysis: stable in neutral and weakly acidic media, in 0.1 N NaOH, 50% hydrolysis occurs in 3.8 h (Hartley & Kidd 1987; Tomlin 1994).
- **Biodegradation:**
- **Biotransformation:**
- **Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:**

Half-Lives in the Environment:
- **Air:**
  - Surface water: photodegradation of vinclozolin aqueous solution (2 ppm), $t_\text{½} = 7$ min and 92 min in the presence of TiO$_2$ (20 ppm), and Fe$_2$O$_3$ (100 ppm), respectively, when irradiated with UV light (Hustert & Moza 1997)
- **Groundwater:**
- **Sediment:**
- **Biota:**
19.1.42 Warfarin

Common Name: Warfarin
Synonym: Coumafen, Zoocoumarin
Chemical Name: 3-(α-acetonylbenzyl)-4-hydroxycoumarin
CAS Registry No: 81-81-2
Use: rodenticide
Molecular Formula: C₁₉H₁₆O₄
Molecular Weight: 308.328
Melting Point (°C): 161 (Lide 2003)
Boiling Point (°C): dec. (Montgomery 1993)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₙₕ (kJ/mol):
Entropy of Fusion, ΔSₙₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₙₕ = 56 J/mol K), F: 0.0463 (mp at 161°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
40 (shake flask, Coon et al. 1954)
17 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
17 (20°C, Montgomery 1993; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
1.55 × 10⁻⁴ (21.5°C, Hartley & Kidd 1987)
9.0 (21.5°C, Worthing & Walker 1987; Tomlin 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
2.86 × 10⁻⁴ (calculated-P/C, Howard 1991)

Octanol/Water Partition Coefficient, log Kₐw:
2.52 (at pH 3, Howard 1991)
3.20 (calculated, Montgomery 1993)

Octanol/Air Partition Coefficient, log Kₐₐₚ:

Bioconcentration Factor, log BCF:
1.68 (calculated, Howard 1991)

Sorption Partition Coefficient, log Kₐₚ:
2.75 (estimated, Howard 1991)
2.96 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: Photooxidation $t_{1/2} = 0.254–1.87$ h was estimated based on rate constants for reaction with hydroxyl radicals and ozone in air (Howard et al. 1991).

Hydrolysis: very slow with a $t_{1/2} = 16$ yr at pH 7; the chemical hydrolysis rate constants, $k = 1.4 \times 10^{-4}$ M$^{-1}$ h$^{-1}$ for acid, neutral-$k = 4.9 \times 10^{-6}$ M$^{-1}$ h$^{-1}$ and $k = 0.026$ M$^{-1}$ h$^{-1}$ for base (Ellington et al. 1988; quoted, Howard 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168–672$ h, anaerobic $t_{1/2} = 672–2688$ h were estimated based on aqueous aerobic biodegradation (Howard et al. 1991).

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

Half-Lives in the Environment:
Air: estimated $t_{1/2} = 11.6$ min due to reaction with photochemically produced hydroxyl radicals and ozone in the vapor phase (Howard 1991);

$\text{H}_{1/2}{\text{Air}} = 0.254–1.87$ h based on estimated photooxidation in air (Howard et al. 1991).

Surface water: $t_{1/2} = 168–672$ h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991);

slow hydrolysis $t_{1/2} = 15$ yr at pH 7 (Howard 1991).

Groundwater: $t_{1/2} = 336–1344$ h based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:
Soil: $t_{1/2} = 168–672$ h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991).

Biota:
Common Name: Zineb
Synonym: Dithane Z-78, Parzate Zineb, Lonaol, Aspor
Chemical Name: zinc ethylene-1,2-bisdithiocarbamate
CAS Registry No: 12122-67-7
Uses: fungicide
Molecular Formula: \((\text{C}_4\text{H}_6\text{N}_2\text{S}_4\text{Zn})_n\)
Molecular Weight: \((275.773)_n\)
Melting Point (°C):
decomposes without melting (Worthing & Walker 1983)
\[157\] (dec., Tomlin 1994; Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant \(pK_a\):
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), \(F\): 0.0507 (mp at 157°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
\[1\] (Melnikov 1971)
\[10\] (Spencer 1982)
\[10\] (room temp., Tomlin 1994)
Vapor Pressure (Pa at 25°C or as indicated):
negligible at rm. temp. (Worthing & Walker 1983)
\[1.07 \times 10^{-5}\] (20°C, quoted, Howard 1991)
\[< 1 \times 10^{-5}\] (20°C, Hartley & Kidd 1987; Tomlin 1994)
\[1.0 \times 10^{-5}\] (10–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, \(\log K_{OW}\):
\[\leq 1.30\] (Tomlin 1994)
Octanol/Air Partition Coefficient, \(\log K_{OA}\):
Bioconcentration Factor, \(\log BCF\):
\[2.11, 2.23, < 1.0,\] (activated sludge, algae, Golden ide, Freitag et al. 1985)
\[2.28\] (calculated-S, Kenaga 1980b; quoted, Howard 1991)
Sorption Partition Coefficient, \(\log K_{OC}\):
\[3.08\] (soil, calculated-S, Kenaga 1980b; quoted, Howard 1991)
\[3.0\] (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
Photolysis: unstable to light, moisture and heat on prolonged storage (Tomlin 1994).
Fungicides

Half-Lives in the Environment:

Air: \( t_{\frac{1}{2}} = 11–14 \) d in greenhouse experiment, microagroecosystem chambers (Nash & Beall 1980);
\( t_{\frac{1}{2}} = 11–14 \) d by gravitational settling and degradation (Howard 1991).

Surface water:

Groundwater:

Sediment:

Soil: \( t_{\frac{1}{2}} = 23 \) d in 1-cm surface soil (sandy loam with pH 6.7), greenhouse experiment in microagroecosystem chambers (Nash & Beall 1980);
\( t_{\frac{1}{2}} = 16–23 \) d upper layer of soil (Howard 1991);
field \( t_{\frac{1}{2}} \approx 30 \) d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota: \( t_{\frac{1}{2}} = 14 \) d on tomato leaves, green house experiment, microagroecosystem chambers (Nash & Beall 1980);
\( t_{\frac{1}{2}} = 7 \) d for tomato fruit in the field, \( t_{\frac{1}{2}} = 3.4 \) d for soybean leaves and \( t_{\frac{1}{2}} = 9 \) d for tomatoes (Nash 1983);
\( t_{\frac{1}{2}} = 14 \) d for tomato leaves, \( t_{\frac{1}{2}} = 7 \) d for tomatoes, \( t_{\frac{1}{2}} = 11 \) d for lettuce and \( t_{\frac{1}{2}} = 35 \) d for grapes (Howard 1991).
19.1.44 Ziram

Common Name: Ziram
Synonym: Aaprotect, Fuklasin, Zerlate, zirmane
Chemical Name: zinc bis(dimethyldithiocarbamate)
CAS Registry No: 137-30-4
Uses: fungicide, bird and rodent repellent
Molecular Formula: C₆H₁₂N₂S₄Zn
Molecular Weight: 305.841
Melting Point (°C):
250 (Howard 1991; Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
2.00 (Spencer 1982)
Molar Volume (cm³/mol):
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔHₚₜ (kJ/mol):
Entropy of Fusion, ΔSₚₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₜ = 56 J/mol K), F: 0.0062 (mp at 250°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
65 (Melnikov 1971)
65 (Martin & Worthing 1977; Worthing & Walker 1983, 1987)
4.0 (20°C, Spencer 1982)
65 (Hartley & Kidd 1987)
0.03 (20°C, Tomlin 1994)
65 (Milne 1995)
Vapor Pressure (Pa at 25°C or as indicated):
< 1 × 10⁻⁶ (extrapolated, Tomlin 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_OW:
1.086 (Tomlin 1994)
Octanol/Air Partition Coefficient, log K_OA:
Bioconcentration Factor, log BCF:
1.77 (calculated-S, Kenaga 1980b; quoted, Howard 1991)
Sorption Partition Coefficient, log K_OC:
2.64 (soil, calculated-solubility, Kenaga 1980b; quoted, Howard 1991)
2.60 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
Environmental Fate Rate Constants, k, or Half-Lives, tₜₛ:
Hydrolysis: decomposed in acidic media (Tomlin 1994).
Half-Lives in the Environment:

Air:
Surface water: decomposed in acidic media, and by UV irradiation (Tomlin 1994).

Groundwater:

Sediment:
Soil: field $t_{1/2} \sim 30$ d (estimated, Augustijn-Beckers et al. 1992; Hornsby et al. 1996).

Biota: for orally administered to rate was mostly eliminated within 1–2 d (Tomlin 1994).
### Table 19.2.1
Common names, chemical names and physical properties of fungicides

<table>
<thead>
<tr>
<th>Name</th>
<th>Synonym</th>
<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>pK_a</th>
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<tbody>
<tr>
<td>Anilazine [101-05-3]</td>
<td>Botrysan, Direz, Dyren</td>
<td>2-chloro-N-(4,6-dichloro-1,3,5-triazin-2-yl)aniline</td>
<td>C₉H₅Cl₃N₄</td>
<td>275.522</td>
<td>160</td>
<td>0.0474</td>
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<td>Benodanil [15310-01-8]</td>
<td>Calirux</td>
<td>2-iodo-N-phenylbenzamide</td>
<td>C₁₃H₁₀INO</td>
<td>323.129</td>
<td>137</td>
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<td>Benomyl [17804-35-2]</td>
<td>Benlate</td>
<td>methyl 1-(butylcarbamoyl)benz-imidazol-2-ylcarbamate</td>
<td>C₁₃H₁₀N₂O₃</td>
<td>390.318</td>
<td>140</td>
<td>0.0744</td>
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<td>Bicarbonate [70585-36-3]</td>
<td>Baycor, Baymat, Biloxa, Sibutol</td>
<td>1-(biphenyl-4-yloxy)-3,3-dimethyl-1H-1,2,4-triazol-1-yl)butan-2-ol</td>
<td>C₂₀H₂₃N₃O₂</td>
<td>337.415</td>
<td>118</td>
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<td>diastereoisomer A</td>
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<td>diastereoisomer B</td>
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<td>[55179–31–2]</td>
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<td>Buprimate [41483-43-6]</td>
<td>Nimrod, Nimrod T</td>
<td>5-butyl-2-ethylamino-6-methyl-pyrimidinyl dimethylsulfamate</td>
<td>C₁₃H₂₃N₄O₅</td>
<td>361.419</td>
<td>50–51</td>
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<td>Captan [133-06-2]</td>
<td>Aacaption, Amercide, Captab, orthocide</td>
<td>N-trichloromethylthio-4-cyclohexene-1,2-dicarboximide</td>
<td>C₉H₁₀Cl₂NO₂</td>
<td>300.590</td>
<td>172.5</td>
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<td>Carbenzazim [10605-21-7]</td>
<td>Bavistin, BCM, Carbenzal</td>
<td>carbamic acid, methyl-1H-benzimidazol-2-yl</td>
<td>C₁₂H₁₀N₂O₂</td>
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<td>Carboxin [5234-68-4]</td>
<td>Vitavac, carbathein</td>
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<td>Chloroneb [2675-77-6]</td>
<td>Tersan SP</td>
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<td>235.302</td>
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<td>Chloropricin [76-06-2]</td>
<td>Nitrochloroform</td>
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<td>Chlorothalonin [1897-45-6]</td>
<td>Bravo, Daconil</td>
<td>2,4,6-tetrachloro-1,3-benzene-dicarbonitrile</td>
<td>C₁₂H₁₀N₂O₂</td>
<td>265.911</td>
<td>250</td>
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<td>Dazomet (Fum.) [533-74-4]</td>
<td>Salvo, Mylone, Basamid</td>
<td>3,5-dimethyl-1,3,5-thiadiazin-2-thione</td>
<td>C₁₂H₁₀N₂O₂</td>
<td>162.276</td>
<td>106</td>
<td>0.16</td>
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<td>Dichlofluanid [1085-98-9]</td>
<td>Euaren, Elvaron</td>
<td>N-dichlorofluoroethylthio-N,N'-dimethyl-N'-phenylsulfamide</td>
<td>C₁₀H₁₀Cl₂F₂N₂O₂S₂</td>
<td>333.229</td>
<td>105.3</td>
<td>0.163</td>
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<td>Dichlone [117–80–6]</td>
<td>Phygon</td>
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<td>227.044</td>
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<td>Dicofol [115–32–2]</td>
<td>Kelthan</td>
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<td>370.485</td>
<td>77.5</td>
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<td>Dithianon [3347-22-6]</td>
<td>Delan</td>
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<td>296.324</td>
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<td><strong>Fungicides</strong></td>
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<td><strong>Edifenphos [17109-49-8]</strong></td>
<td>EDDP, Hinosan</td>
<td>O-ethyl S,S-diphenyl-phosphoradithioate</td>
<td>C_{14}H_{15}O_2PS_2</td>
<td>310.371</td>
<td>-25</td>
<td>1</td>
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<td><strong>Ethirimol [23947-60-6]</strong></td>
<td>ethazol, ethazole, Terazole</td>
<td>5-butyl-2-ethylamino-6-methyl-pyrimidin-4-ol</td>
<td>C_{10}H_{13}N_3O</td>
<td>209.288</td>
<td>160</td>
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<td><strong>Etridiazole [2593-15-9]</strong></td>
<td>Biloc, Rimidin, Rubigan</td>
<td>ethyl 3-trichloromethyl-1,2,4-triadiazolyl ether</td>
<td>C_{14}H_{14}N_2O</td>
<td>247.530</td>
<td>19.9</td>
<td>1</td>
<td>2.27</td>
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<td><strong>Fenarimol [60168-88-9]</strong></td>
<td>fenfurame</td>
<td>(±)-2,4-dichloro-α-(pyrimidin-5-yl) benzhydryl alcohol</td>
<td>C_{12}H_{11}Cl_2N_2O</td>
<td>331.195</td>
<td>118</td>
<td>0.122</td>
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<td><strong>Fenfuram [24691-80-3]</strong></td>
<td>Corbel, Mitril</td>
<td>2-methyl-3-fruanilide</td>
<td>C_{11}H_{16}N_3O</td>
<td>201.221</td>
<td>109–110</td>
<td>0.148</td>
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<td><strong>Fenpropimorph [67564-91-4]</strong></td>
<td>Corbel, Mistral</td>
<td>(±)-cis-4-[3-(4-tert-butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine</td>
<td>C_{20}H_{33}NO</td>
<td>303.482</td>
<td>oil</td>
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<td>6.98</td>
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<td><strong>Folpet [133-07-3]</strong></td>
<td>Foltan, Folpan, Folpel, Spolacid</td>
<td>N-(trichloromethylthio)phthalimide</td>
<td>C_{9}H_{4}Cl_3NO_2S</td>
<td>296.558</td>
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<td><strong>Formaldehyde [50-00-0]</strong></td>
<td>Formalin, methanal</td>
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<td>HCHO</td>
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<td><strong>Furalaxyl [57646-30-7]</strong></td>
<td>Fongarid</td>
<td>methyl-N-(2-furoyl)-N-(2,6-xylyl)-DL-alaninate</td>
<td>C_{15}H_{21}NO_4</td>
<td>301.337</td>
<td>70</td>
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<td><strong>Hexachlorobenzene [118–74-1]</strong></td>
<td>HCB</td>
<td>hexachlorobenzene</td>
<td>C_{6}Cl_6</td>
<td>284.782</td>
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<td><strong>Imazalil [35554-44-0]</strong></td>
<td>Bromazil, Deccoziel</td>
<td>(±)-1-(β-allyloxy-2,4-dichlorophenyl)-ethylimidazole</td>
<td>C_{10}H_{15}ClN_2O</td>
<td>297.179</td>
<td>50</td>
<td>0.568</td>
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<td><strong>Iprobenfos [26087-47-8]</strong></td>
<td>Kitazin</td>
<td>S-benzylo,O,O-di-isopropyl phosphoro-thioate</td>
<td>C_{13}H_{21}O_3PS</td>
<td>288.342</td>
<td>oil</td>
<td>1</td>
<td>192–194 dec</td>
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<td><strong>Mancozeb [8018–01–7]</strong></td>
<td>Dithane ultra, Dithane M45</td>
<td>manganese ethylenebis(dithiocarbamate)</td>
<td>(C_{12}H_{13}MnN_2S_4)_x</td>
<td>(265.302)_x</td>
<td>dec 200</td>
<td>0.354</td>
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<td><strong>Maneb [12427–38–2]</strong></td>
<td>MEB, Dithane, Bravo</td>
<td>methyl N-(2-methoxyacetyl)-2,6-xylyl)-DL-alaninate</td>
<td>C_{15}H_{21}NO_4</td>
<td>279.333</td>
<td>71</td>
<td>0.354</td>
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<td><strong>Metalaxyl [57837-19-1]</strong></td>
<td>Ridomil, Apron Fulbol</td>
<td>zinc ammoniate ethylenebisdithio-carbamate-poly(ethylenethiurmdisulfide)</td>
<td>C_{13}H_{21}NO_4</td>
<td>230.907</td>
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<td><strong>Metiram [9006-42-4]</strong></td>
<td>Carbatene, Polyram</td>
<td>2-chloro-6-(trichloromethyl)pyridine</td>
<td>C_{6}H_{4}ClN</td>
<td>267.301</td>
<td>129</td>
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<td><strong>Nitrapyrin [1929–82–4]</strong></td>
<td>Plantvax</td>
<td>2,6-dihydro-2-methyl-1,4-oxathi-3-carboxanilide 4,4-dioxide</td>
<td>C_{6}H_{4}ClNO_S</td>
<td>284.184</td>
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<td><strong>Penconazole [66246-88-6]</strong></td>
<td>Topas, Topaz, Topaze</td>
<td>1-(2,4-dichloro-β-propylphenyl-ethyl)-1H,1,2,4-triazole</td>
<td>C_{13}H_{15}Cl_2N_3</td>
<td>284.184</td>
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<td>0.454</td>
<td>1.51</td>
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<td><strong>Procymidone [32809-16-8]</strong></td>
<td>Sumisclex, Sumilex</td>
<td>N-(3,5-dichlorophenyl)-1,2-dimethyl-cyclopropene-1,2-dicarboximide</td>
<td>C_{13}H_{11}Cl_2NO_2</td>
<td>284.138</td>
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<td>0.0414</td>
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<td><strong>Propargite [2312–35–8]</strong></td>
<td>Comite, Omite</td>
<td>2-[(1,1-dimethylethyl)phenoxy] cyclohexyl 2-propynyl sulfite</td>
<td>C_{8}H_{24}O_S</td>
<td>360.472</td>
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<td><strong>Propiconazole [60207-90-1]</strong></td>
<td>(±)-1-[2,4-(dichlorophenyl)-4-propyl-1,3-dioxolan-2-methyl]-</td>
<td>C_{15}H_{17}Cl_2N_3O_2</td>
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<td>liquid</td>
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<td>1.09</td>
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<th>Name</th>
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<th>Chemical name</th>
<th>Molecular formula</th>
<th>Molecular weight, MW (g/mol)</th>
<th>m.p. (°C)</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>pKₐ</th>
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<td>Quintozene [82-68-8]</td>
<td>Tritisan, Botrillex, Terraclor</td>
<td>pentachloronitrobenzene</td>
<td>C₆Cl₅NO₂</td>
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<td>Tecnazene [117-18-0]</td>
<td>Folosan, Fusarex</td>
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<td>Mertect, Storite</td>
<td>2-(thiazol-4-yl)benzimidazole</td>
<td>C₉H₇N₃S</td>
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<td>Thiophanate-methyl</td>
<td>Topsin M, Mildothane</td>
<td>dimethyl 4,4’-(o-phenylene)bis(3-thioallphanate)</td>
<td>C₁₂H₁₄N₄O₄S₂</td>
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<td>0.0361 7.28</td>
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<td>Thiram [137-26-8]</td>
<td>Arasan, Tersan, Fernasan</td>
<td>tetramethylthiuram disulphide</td>
<td>C₆H₁₂N₄S₄</td>
<td>240.432</td>
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<td>Tolclofos-methyl</td>
<td>Rizolex</td>
<td>O-2,6-dichloro-p-tolylo,O,O-dimethyl phosphorothioate</td>
<td>C₁₀H₁₇Cl₂O₂PS</td>
<td>301.127</td>
<td>78-80</td>
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<td>Tolyfluanid [731-27-1]</td>
<td>Euparen M</td>
<td>N-dichlorofluoromethylthio-N,N'-dimethyl-N-p-tolysulphamide</td>
<td>C₁₆H₁₇Cl₂FN₂O₂S₂</td>
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<td>Triadimefon [43121-43-3]</td>
<td>Amiral, Bayeton</td>
<td>1-((chlorophenoxy)-3,3-dimethyl-1-1H-1,2,4-triazol-1-yl)butanone</td>
<td>C₁₄H₁₆ClIN₃O₂</td>
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<td>Baytan</td>
<td>1-(4-chlorophenoxy)-3,3-dimethyl-1-((1H-1,2,4-triazol-1-yl)butan-2-ol</td>
<td>C₁₄H₁₆ClIN₃O₂</td>
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<td>Beam, Bim, Blascide</td>
<td>5-methyl-1,1,2,4-triazol-3-[4,5-]benzothiazole</td>
<td>C₁₀H₇N₃S</td>
<td>189.237</td>
<td>187</td>
<td>0.0257 0.419 3.70</td>
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<tr>
<td>Triflumizole [99387–89-0]</td>
<td>Trifmine</td>
<td>(E)-4-chloro-α,α,α-trifluoro-N-(1-imidazol-1-yl-propoxyethylidene)-o-toluidine</td>
<td>C₁₄H₁₃ClF₃N₃O</td>
<td>345.747</td>
<td>63.5</td>
<td>0.419 3.70</td>
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<td>Triforine [26644-46-2]</td>
<td></td>
<td>1,4-bis(2,2,2-trichloro-1-formamido-ethyl)piperazine</td>
<td>C₁₀H₈Cl₂N₄O₂</td>
<td>434.962</td>
<td>155 dec</td>
<td>0.0530</td>
<td></td>
</tr>
<tr>
<td>Vinclozolin [50471-44-8]</td>
<td>Ronilan</td>
<td>(RS)-1-(3-(5,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione</td>
<td>C₁₀H₈Cl₂NO₃</td>
<td>286.110</td>
<td>108</td>
<td>0.153</td>
<td></td>
</tr>
<tr>
<td>Warfarin (R.) [81-81-2]</td>
<td>Coumarin Dethmor</td>
<td>4-hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one</td>
<td>C₁₀H₁₀O₄</td>
<td>308.328</td>
<td>161</td>
<td>0.0463</td>
<td></td>
</tr>
<tr>
<td>Zineb [12122-67-7]</td>
<td>Zinebe</td>
<td>zine ethylenebis(dithiocarbamate)</td>
<td>C₁₂H₁₃N₃S₄Zn</td>
<td>275.773</td>
<td>157 dec</td>
<td>0.0507</td>
<td></td>
</tr>
<tr>
<td>Ziram [137-30-4]</td>
<td>Zirame</td>
<td>zine bis(dimethylthiocarbamate)</td>
<td>C₁₂H₁₃N₃S₄Zn</td>
<td>305.841</td>
<td>250</td>
<td>0.0062</td>
<td></td>
</tr>
</tbody>
</table>

Note: Fum.—fumigant, I.—insecticide, R.—rodenticide

* Assuming ∆Sₘₚ = 56 J/mol K
## TABLE 19.2.2
Summary of selected physical-chemical properties of fungicides at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry's law constant</th>
<th>log K_{OC} reported</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P{\text{V}}/Pa</td>
<td>P{\text{L}}/Pa</td>
<td>S/(g/m{\text{3}})</td>
<td>C{\text{S}}/(mol/m{\text{3}})</td>
</tr>
<tr>
<td>Anilazine</td>
<td>8.20 × 10{\text{–7}}</td>
<td>1.77 × 10{\text{–5}}</td>
<td>8</td>
<td>0.0290</td>
</tr>
<tr>
<td>Benalaxyl</td>
<td>0.00133</td>
<td>4.65 × 10{\text{–3}}</td>
<td>37</td>
<td>0.1137</td>
</tr>
<tr>
<td>Benodanil</td>
<td>1.00 × 10{\text{–8}}</td>
<td>1.28 × 10{\text{–7}}</td>
<td>2</td>
<td>0.0062</td>
</tr>
<tr>
<td>Benomyl</td>
<td>1.33 × 10{\text{–6}}</td>
<td>1.82 × 10{\text{–7}}</td>
<td>9</td>
<td>0.0069</td>
</tr>
<tr>
<td>Bitertanol</td>
<td>1.00 × 10{\text{–6}}</td>
<td>8.31 × 10{\text{–6}}</td>
<td>5</td>
<td>0.0118</td>
</tr>
<tr>
<td>diastereoisomer A</td>
<td>2.20 × 10{\text{–6}}</td>
<td>8.10 × 10{\text{–6}}</td>
<td>2.9</td>
<td>0.0069</td>
</tr>
<tr>
<td>diastereoisomer B</td>
<td>2.50 × 10{\text{–6}}</td>
<td>3.86 × 10{\text{–6}}</td>
<td>1.6</td>
<td>0.0038</td>
</tr>
<tr>
<td>Bupirimate</td>
<td>0.00067</td>
<td>1.21 × 10{\text{–3}}</td>
<td>22</td>
<td>0.0695</td>
</tr>
<tr>
<td>Captan</td>
<td>1.10 × 10{\text{–5}}</td>
<td>4.23 × 10{\text{–4}}</td>
<td>5.1</td>
<td>0.0170</td>
</tr>
<tr>
<td>Carboxin</td>
<td>6.50 × 10{\text{–5}}</td>
<td>3.82 × 10{\text{–5}}</td>
<td>8</td>
<td>0.0418</td>
</tr>
<tr>
<td>Chloroneb</td>
<td>1.30 × 10{\text{–5}}</td>
<td>5.98 × 10{\text{–5}}</td>
<td>195</td>
<td>0.829</td>
</tr>
<tr>
<td>Chloropicrin (I,Fum.)</td>
<td>2400</td>
<td>2400</td>
<td>2270</td>
<td>13.81</td>
</tr>
<tr>
<td>Chlorothalonil</td>
<td>0.133*</td>
<td>22.86</td>
<td>0.6</td>
<td>0.0023</td>
</tr>
<tr>
<td>Dazomet (Fum.)</td>
<td>4.0 × 10{\text{–4}}</td>
<td>2.47 × 10{\text{–3}}</td>
<td>3000</td>
<td>18.48</td>
</tr>
<tr>
<td>Dichlofluanid</td>
<td>2.10 × 10{\text{–5}}</td>
<td>1.32 × 10{\text{–4}}</td>
<td>1.3</td>
<td>0.0039</td>
</tr>
<tr>
<td>Dithianon</td>
<td>6.60 × 10{\text{–5}}</td>
<td>6.28 × 10{\text{–4}}</td>
<td>0.5</td>
<td>0.0017</td>
</tr>
<tr>
<td>Edifenphos</td>
<td>0.013</td>
<td>0.013</td>
<td>56</td>
<td>0.180</td>
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<tr>
<td>Ethirimol</td>
<td>2.67 × 10{\text{–4}}</td>
<td>5.78 × 10{\text{–3}}</td>
<td>200</td>
<td>0.956</td>
</tr>
<tr>
<td>Etridiazole</td>
<td>0.013</td>
<td>0.013</td>
<td>50</td>
<td>0.202</td>
</tr>
<tr>
<td>Fenamidol</td>
<td>2.93 × 10{\text{–5}}</td>
<td>2.44 × 10{\text{–4}}</td>
<td>14</td>
<td>0.0423</td>
</tr>
<tr>
<td>Fenfuram</td>
<td>2.0 × 10{\text{–5}}</td>
<td>1.39 × 10{\text{–4}}</td>
<td>100</td>
<td>0.497</td>
</tr>
<tr>
<td>Fenpropimorph</td>
<td>0.0023</td>
<td>2.30 × 10{\text{–3}}</td>
<td>4.3</td>
<td>0.0142</td>
</tr>
<tr>
<td>Folpet</td>
<td>0.0013</td>
<td>0.0414</td>
<td>1</td>
<td>0.0034</td>
</tr>
<tr>
<td>Formaldehyde</td>
<td>&gt; 1 atm</td>
<td>miscible</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Furalaxyl</td>
<td>230</td>
<td></td>
<td>763</td>
<td>2.127</td>
</tr>
<tr>
<td>Imazalil</td>
<td>9.30 × 10{\text{–6}}</td>
<td>1.75 × 10{\text{–5}}</td>
<td>1400</td>
<td>4.71</td>
</tr>
<tr>
<td>Metalaxyl</td>
<td>7.47 × 10{\text{–4}}</td>
<td>2.18 × 10{\text{–3}}</td>
<td>8400</td>
<td>30.08</td>
</tr>
<tr>
<td>Metiram</td>
<td>&lt; 0.00001</td>
<td></td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Oxydicarboxin</td>
<td>0.00133</td>
<td>0.0139</td>
<td>1000</td>
<td>3.741</td>
</tr>
<tr>
<td>Penconazole</td>
<td>0.00021</td>
<td>4.66 × 10{\text{–4}}</td>
<td>73</td>
<td>0.257</td>
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(Continued)
TABLE 19.2.2 (Continued)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure</th>
<th>Solubility</th>
<th>Henry's law constant</th>
<th>log KOC</th>
<th>log KoC reported</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P^v/Pa</td>
<td>P^l/Pa</td>
<td>S/(g/m^3)</td>
<td>C^l/(mol/m^3)</td>
<td>C^l^(mol/m^3)</td>
</tr>
<tr>
<td>Procymidone</td>
<td>0.0187</td>
<td>0.4534</td>
<td>4.5</td>
<td>0.0158</td>
<td>0.384</td>
</tr>
<tr>
<td>Propiconazole</td>
<td>5.60 × 10^{-5}</td>
<td>5.60 × 10^{-5}</td>
<td>110</td>
<td>0.321</td>
<td>0.321</td>
</tr>
<tr>
<td>Quintozene</td>
<td>0.0066</td>
<td>0.104</td>
<td>0.44</td>
<td>0.0015</td>
<td>0.023</td>
</tr>
<tr>
<td>Tecnazene</td>
<td></td>
<td></td>
<td>0.44</td>
<td>0.0017</td>
<td>0.0091</td>
</tr>
<tr>
<td>Thiabendazole</td>
<td>5.33 × 10^{-2}</td>
<td>3.13 × 10^{-4}</td>
<td>50</td>
<td>0.249</td>
<td>146.1</td>
</tr>
<tr>
<td>Thiophanate-methyl</td>
<td>1.30 × 10^{-5}</td>
<td>3.70 × 10^{-4}</td>
<td>3.5</td>
<td>0.0102</td>
<td>0.291</td>
</tr>
<tr>
<td>Thiram</td>
<td>0.00133</td>
<td>0.0209</td>
<td>30</td>
<td>0.125</td>
<td>1.963</td>
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<tr>
<td>Tolclofos-methyl</td>
<td>0.0573</td>
<td>0.196</td>
<td>0.3</td>
<td>0.001</td>
<td>0.0034</td>
</tr>
<tr>
<td>Tolyfluquin</td>
<td>1.6 × 10^{-5}</td>
<td>8.06 × 10^{-5}</td>
<td>0.9</td>
<td>0.0026</td>
<td>0.0131</td>
</tr>
<tr>
<td>Triadimefon</td>
<td>2.0 × 10^{-6}</td>
<td>7.37 × 10^{-6}</td>
<td>71.5</td>
<td>0.243</td>
<td>0.897</td>
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<tr>
<td>Triadimenol</td>
<td>4.13 × 10^{-8}</td>
<td>4.03 × 10^{-7}</td>
<td>47</td>
<td>0.159</td>
<td>1.549</td>
</tr>
<tr>
<td>diastereoisomer A</td>
<td>&lt; 0.001</td>
<td></td>
<td>62</td>
<td>0.210</td>
<td>2.761</td>
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<tr>
<td>diastereoisomer B</td>
<td>4.10 × 10^{-8}</td>
<td>4.85 × 10^{-7}</td>
<td>32</td>
<td>0.108</td>
<td>1.280</td>
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<tr>
<td>Tricyclazole</td>
<td>2.67 × 10^{-5}</td>
<td>1.09 × 10^{-3}</td>
<td>1600</td>
<td>8.46</td>
<td>346.2</td>
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<tr>
<td>Triflumizole</td>
<td>1.47 × 10^{-6}</td>
<td>3.53 × 10^{-6}</td>
<td>12500</td>
<td>36.16</td>
<td>86.90</td>
</tr>
<tr>
<td>Triforine</td>
<td>2.67 × 10^{-5}</td>
<td>5.16 × 10^{-4}</td>
<td>30</td>
<td>0.069</td>
<td>1.332</td>
</tr>
<tr>
<td>Vinclozolin</td>
<td>1.33 × 10^{-5}</td>
<td>8.81 × 10^{-5}</td>
<td>1000</td>
<td>3.495</td>
<td>23.14</td>
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<tr>
<td>Warfarin (R.)</td>
<td>1.55 × 10^{-4}</td>
<td>3.43 × 10^{-3}</td>
<td>17</td>
<td>0.0551</td>
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<tr>
<td>Zineb</td>
<td>1.33 × 10^{-5}</td>
<td></td>
<td>10</td>
<td>0.0363</td>
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<tr>
<td>Ziram</td>
<td>1.0 × 10^{-6}</td>
<td>1.53 × 10^{-4}</td>
<td>65</td>
<td>0.213</td>
<td>32.61</td>
</tr>
</tbody>
</table>

Note: * The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
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<tbody>
<tr>
<td>Benomyl</td>
<td>1</td>
<td>4</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>Captan</td>
<td>2</td>
<td>2</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Chloropicrin</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Chlorothalonil</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Thiram</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
</tbody>
</table>

<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>
19.3 REFERENCES


Fungicides


Singh, R.P., Chiba, M. (1985) Solubility of benomyl in water at different pHs and its conversion to methyl 2-benzimidazolecarbamate,
Siebers, J., Gottschild, D., Notting, H.-G. (1994) Pesticides in precipitation in Northern Germany...


### Appendix 1

#### 1.1 LIST OF SYMBOLS AND ABBREVIATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>( A_i )</td>
<td>area of phase ( i ), m(^2)</td>
</tr>
<tr>
<td>ALPM</td>
<td>automated log-P measurement</td>
</tr>
<tr>
<td>AS</td>
<td>absorption spectrophotometry</td>
</tr>
<tr>
<td>BCF</td>
<td>bioconcentration factor</td>
</tr>
<tr>
<td>bp</td>
<td>boiling point, °C</td>
</tr>
<tr>
<td>C</td>
<td>molar concentration, mol/L or mmol/m(^3)</td>
</tr>
<tr>
<td>( C^S )</td>
<td>saturated aqueous concentration, mol/L or mmol/m(^3)</td>
</tr>
<tr>
<td>( C_l )</td>
<td>liquid or supercooled liquid concentration, mol/L or mmol/m(^3)</td>
</tr>
<tr>
<td>( C_s )</td>
<td>solid molar concentration, mol/L or mmol/m(^3)</td>
</tr>
<tr>
<td>( C_A )</td>
<td>concentration in air phase, mol/L or mmol/m(^3)</td>
</tr>
<tr>
<td>( C_W )</td>
<td>concentration in water phase, mol/L or mmol/m(^3)</td>
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<tr>
<td>(^{14})C</td>
<td>radioactive labelled carbon-14 compound</td>
</tr>
<tr>
<td>CC</td>
<td>countercurrent chromatography</td>
</tr>
<tr>
<td>COD</td>
<td>chemical oxygen demand</td>
</tr>
<tr>
<td>CPC</td>
<td>centrifugal partition chromatography</td>
</tr>
<tr>
<td>D</td>
<td>D values, mol/Pa·h</td>
</tr>
<tr>
<td>( D_A )</td>
<td>D values for advection, mol/Pa·h</td>
</tr>
<tr>
<td>( D_{Ai} )</td>
<td>D values for advective loss in phase ( i ), mol/Pa·h</td>
</tr>
<tr>
<td>( D_R )</td>
<td>D value for reaction, mol/Pa-h</td>
</tr>
<tr>
<td>( D_{Ri} )</td>
<td>D value for reaction loss in phase ( i ), mol/Pa-h</td>
</tr>
<tr>
<td>( D_{ij} )</td>
<td>intermedia D values, mol/Pa-h</td>
</tr>
<tr>
<td>( D_{IVW} )</td>
<td>intermedia D value for air-water diffusion (absorption), mol/Pa-h</td>
</tr>
<tr>
<td>( D_{RW} )</td>
<td>intermedia D value for air-water dissolution, mol/Pa-h</td>
</tr>
<tr>
<td>( D_{AQW} )</td>
<td>D value for total particle transport (dry and wet), mol/Pa-h</td>
</tr>
<tr>
<td>( D_{RS} )</td>
<td>D value for rain dissolution (air-soil), mol/Pa-h</td>
</tr>
<tr>
<td>( D_{QS} )</td>
<td>D value for wet and dry deposition (air-soil), mol/Pa-h</td>
</tr>
<tr>
<td>( D_{VS} )</td>
<td>D value for total soil-air transport, mol/Pa-h</td>
</tr>
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<td>( D_S )</td>
<td>D value for air-soil boundary layer diffusion, mol/Pa-h</td>
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<td>( D_{SW} )</td>
<td>D value for water transport in soil, mol/Pa-h</td>
</tr>
<tr>
<td>( D_{SA} )</td>
<td>D value for air transport in soil, mol/Pa-h</td>
</tr>
<tr>
<td>( D_{Ti} )</td>
<td>total transport D value in bulk phase ( i ), mol/Pa-h</td>
</tr>
<tr>
<td>DOC</td>
<td>dissolved organic carbon</td>
</tr>
<tr>
<td>DOM</td>
<td>dissolved organic matter</td>
</tr>
<tr>
<td>DSC</td>
<td>differential scanning calorimetry</td>
</tr>
<tr>
<td>DTA</td>
<td>differential thermal analyzer</td>
</tr>
<tr>
<td>E</td>
<td>emission rate, mol/h or kg/h</td>
</tr>
<tr>
<td>EPICS</td>
<td>equilibrium partitioning in closed system</td>
</tr>
<tr>
<td>F</td>
<td>fugacity ratio</td>
</tr>
<tr>
<td>( f )</td>
<td>fugacity, Pa</td>
</tr>
<tr>
<td>( f_i )</td>
<td>fugacity in pure phase ( i ), Pa</td>
</tr>
<tr>
<td>f-const.</td>
<td>fragmental constants</td>
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</table>
fluor. fluorescence method
G advective inflow, m³/h
Gₘ advective inflow to bottom sediment m³/h
ΔG Gibbs’s free energy of vaporization kJ/mol or kcal/mol
GC gas chromatography
GC/FID GC analysis with flame ionization detector
GC/ECD GC analysis with electron capture detector
GC-RT GC retention time
gen. col. generator-column
H, HLC Henry’s law constant, Pa·m³/mol, or atm m³/mol
ΔH_fus enthalpy of fusion, kJ/mol
ΔH_sbf enthalpy of sublimation, kJ/mol
ΔH_v enthalpy of vaporization, kJ/mol or kcal/mol
HPLC high pressure liquid chromatography
HPLC/MS HPLC analysis with mass spectrometer detector
HPLC/UV HPLC analysis with UV detector
HPLC/fluo. HPLC analysis with fluorescence detector
HPLC-k’ HPLC-capacity factor correlation
HPLC-RI HPLC-retention index correlation
HPLC-RT HPLC-retention time correlation
HPLC-RV HPLC-retention volume correlation
IP ionization potential
IR infrared absorption
J intermediate quantities for fugacity calculation
K Kjeldahl method
k reaction rate constant
k_i first-order rate constant in phase i, h⁻¹
k_A air/water mass transfer coefficient, air-side, m/h
k_W air/water mass transfer coefficient, water-side, m/h
K_AR/W aerosol/water partition coefficient
K_AW dimensionless air/water partition coefficient
k_d Henry’s law constant with units of vapor pressure
K_a bioconcentration factor
K_s association coefficient
K_OC organic-carbon sorption partition coefficient
K_OM organic-matter sorption partition coefficient
K_OA octanol/air partition coefficient
K_OW octanol/water partition coefficient
K_SDW sediment-water partition coefficient
K_SSDW suspended sediment/water partition coefficient
K_SW soil/water partition coefficient
K_D or K_d sorption coefficient
k_1 uptake/accumulation rate constant, d⁻¹ (day⁻¹)
k_2 elimination/clearance/depuration rate constant, d⁻¹
k_h biodegradation rate constant, d⁻¹
k_n hydrolysis rate constant, d⁻¹
k_p photolysis rate constant, d⁻¹
k_OH photooxidation rate constant for hydroxyl radical
k_NO3 photooxidation rate constant for NO₃ radical
k_O3 photooxidation rate constant for ozone
L lipid content of fish
LSC liquid scintillation counting
LSS liquid scintillation spectrometry
m amount of chemical in phase i, mol or kg
M total amount of chemical, mol or kg
MCI  molecular connectivity indices
MO  molecular orbital calculation
mp.  melting point, °C
MR  molar refraction
MS  mass spectrometry
MW  molecular weight, g/mol
n_c  number of carbon atoms
n_cl  number of chlorine atoms
P  vapor pressure, Pa (Pascal)
P_L  liquid or supercooled liquid vapor pressure, Pa
P_S  solid vapor pressure, Pa
Q  scavenging ratio
QSAR  quantitative structure-activity relationship
QSPR  quantitative structure-property relationship
RC  Radiochemical method
RP-HPLC  reversed phase high pressure liquid chromatography
RP-TLC  reversed phase thin layer chromatography
S  water solubility, mg/L or g/m³
ΔS_fus  entropy of fusion, J/mol·K or cal/mol·K (e.u.)
S_{octanol}  solubility in octanol
SD  standard deviation
SPARC  a computational expert system that predicts chemical reactivity
t/°C  temperature in degree centigrade
t  residence time, h (hour)
t_o  overall residence time, h
_t_A  advection persistence time, h
_t_B  sediment burial residence time, h
_t_r  reaction persistence time, h
_t_{1/2}  half-life, s, h, min, d, month or yr
T_{ij}  intermedia transport rate, mol/h or kg/h
T  system temperature, K
T_B  boiling point, K
T_M  melting point, K
TLC  thin-layer chromatography
TMV  total molecular volume per molecule, Å³ (Angstrom³)
TN  titration method
TSA  total surface area per molecule, Å²
U_1  air side, air-water MTC (same as k_A), m/h
U_2  water side, air-water MTC (same as k_W), m/h
U_3  rain rate (same as U_p), m/h
U_4  aerosol deposition rate, m/h
U_5  soil-air phase diffusion MTC, m/h
U_6  soil-water phase diffusion MTC, m/h
U_7  soil-air boundary layer MTC, m/h
U_8  sediment-water MTC, m/h
U_9  sediment deposition rate, m/h
U_{10}  sediment resuspension rate, m/h
U_{11}  soil-water run-off rate, m/h
U_{12}  soil-solids run-off rate, m/h
U_B  rain rate, m/h
U_Q  dry deposition velocity, m/h
U_B  sediment burial rate, m/h
UV  UV spectrometry
UNIFAC  UNIQUAC functional group activity coefficients
V_i  volume of pure phase i, m³
$V_S$ volume of bottom sediment, $m^3$

$V_{Bi}$ volume of bulk phase $i$, $m^3$

$V_i$ intrinsic molar volume, $cm^3/mol$

$V_M$ molar volume, $cm^3/mol$

$v_i$ volume fraction of phase $i$

$v_Q$ volume fraction of aerosol

VOC volatile organic chemicals

$W$ molecular mass, $g/mol$

$Z_i$ fugacity capacity of phase $i$, $mol/m^3 Pa$

$Z_{Bi}$ fugacity capacity of bulk phase $i$, $mol/m^3 Pa$

### 1.2 GREEK CHARACTERS

π-const. substituent constants for $K_{ow}$ estimation

$\gamma$ solute activity coefficient

$\gamma_o$ solute activity coefficient in octanol phase

$\gamma_W$ solute activity coefficient in water phase

$\rho_i$ density of pure phase $i$, $kg/m^3$

$\rho_{Bi}$ density of bulk phase $i$, $kg/m^3$

$\chi$ molecular connectivity indices

$\phi_{OC}$ or $f_{OC}$ organic carbon fraction

$\phi_i$ organic carbon fraction in phase $i$
# Appendix 2

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