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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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.

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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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Biographies

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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.

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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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10 Ethers

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### 10.1 LIST OF CHEMICALS AND DATA COMPILATIONS

#### 10.1.1 ALIPHATIC ETHERS

#### 10.1.1.1 Dimethyl ether (Methyl ether)

- **Common Name:** Dimethyl ether
- **Synonym:** methyl ether, oxapropane, oxybismethane
- **Chemical Name:** dimethyl ether, methyl ether,
- **CAS Registry No:** 115-10-6
- **Molecular Formula:** C₂H₆O, CH₃OCH₃
- **Molecular Weight:** 46.068
- **Melting Point (°C):**
  - –138.5 (Stull 1947; Stephenson & Malanowski 1987)
  - –141.5 (Riddick et al. 1986; Lide 2003)
- **Boiling Point (°C):**
  - –24.75 (Ambrose et al. 1976)
  - –23.60 (Stephenson & Malanowski 1987)
  - –24.8 (Lide 2003)
- **Density (g/cm³ at 20°C):**
  - 0.6689 (Riddick et al. 1986)
  - 0.6612 (25°C, Riddick et al. 1986)
- **Molar Volume (cm³/mol):**
  - 68.87 (20°C, calculated-density)
  - 60.9 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, ∆Hₜₚ (kJ/mol):**
  - 4.941 (Riddick et al. 1986; Chickos et al. 1999)
- **Entropy of Fusion, ∆Sₜₚ (J/mol K):**
- **Fugacity Ratio at 25°C, F:** 1.0
- **Water Solubility (g/m³ or mg/L at 25°C or as indicated):**
  - 71000 (Seidell 1941; Lange 1971)
  - 35.3% (24°C, selected, Riddick et al. 1986)
  - 65200 (literature data compilation, Yaws et al. 1990)
  - 47480 (calculated-VM, Wang et al. 1992)
- **Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**
  - 100847* (−24.91°C, static method-manometer, measured range −78.22 to −24.91°C, Kennedy et al. 1941)
  - 678090* (calculated-Antoine eq. regression, temp range −115.7 to −23.7°C, Stull 1947)
  - log (P/mmHg) = [−0.2185 × 5409.8/(T/K)] + 7.585479; temp range −115.7 to 125.2°C (Antoine eq., Weast 1972–73)
  - 593300 (Ambrose et al. 1976, Riddick et al. 1986)
  - log (P/kPa) = 6.0823 − 882.52/{(T/K) + 31.90} (Antoine eq., Ambrose et al. 1976)
\[
\log (P_L/kPa) = 6.09354 - 880.813/(–33.007 + T/K); \text{ temp range 241–303 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
\log (P_L/kPa) = 6.28318 - 987.484/(–16.813 + T/K); \text{ temp range 293–360 K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]

\[
\log (P_L/kPa) = 7.48877 - 1971.127/(122.787 + T/K); \text{ temp range 349–400 K (Antoine eq.-VI, Stephenson & Malanowski 1987)}
\]

\[
\]

\[
\log (P/mmHg) = 20.2699 – 1.5914 \times 10^3/(T/K) – 4.653 \cdot \log (T/K) – 1.3178 \times 10^{-10} \cdot (T/K)^2; \text{ temp range 132–400 K (vapor pressure eq., Yaws et al. 1994)}
\]

\[
510000* (20.5°C, vapor-liquid equilibrium, measured range 0.51–120.12°C, Jónasson et al. 1995)
\]

\[
589100 (25.02°C, vapor-liquid equilibrium, measured range 283.12–313.22 K, Bobbo et al. 2000)
\]

\[
596210* (25.022°C, static-pressure sensor, measured range 233–399 K, data fitted to Wagner type eq., Wu et al. 2004)
\]

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

\[
101.0 \text{ (calculated-} 1/K_{AW}, \text{ C}^2_{AW}/\text{CA}, \text{ reported as exptl., Hine & Mookerjee 1975)}
\]

\[
49.5, 105.7 \text{ (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)}
\]

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

0.10 \text{ (shake flask-GC, Leo et al. 1975; Hansch & Leo 1987)}

0.10 \text{ (recommended, Sangster 1989)}

0.10 \text{ (recommended, Hansch et al. 1995)}

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

1.37 \text{ (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)}

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

Oxidation: 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_{SO_2} with O_3 as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{OH} = 5.7 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O}_2(\text{P}) \text{ at room temp. (Gaffney & Levine 1979)}
\]

\[
k_{OH} = 3.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298.9 \text{ K, measured range } 298–505 \text{ K (flash photolysis-resonance fluorescence, Perry et al. 1977)}
\]

\[
k_{OH}(\text{calc}) = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(\text{obs}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)}
\]

\[
k_{NO3} \leq 3.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 2 \text{ K (flash photolysis-visible absorption, Wallington et al. 1986; quoted, Sabljic & Güsten 1990; Atkinson 1991)}
\]

\[
k_{OH} = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K, measured range } 295–442 \text{ K (Tully & Droege 1987)}
\]

\[
k_{NO3} = 2.92 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Sabljic & Güsten 1990)}
\]

\[
k_{OH}(\text{exptl}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 1.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1987)}
\]

\[
k_{OH} = (24.9 \pm 2.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K, measured range } 240–440 \text{ K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)}
\]

\[
k_{OH} = 2.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{soln}} = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)}
\]

\[
k_{OH} = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1990)}
\]

\[
k_{OH} = (2.35 \pm 0.24) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by pulse radiolysis-UV spectroscopy; } k_{OH} = (3.19 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by relative rate method, at } 298 \pm 2 \text{ K (Nelson et al. 1990)}
\]

\[
k_{OH} = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K, measured range } 295–650 \text{ K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)}
\]
$k_{\text{OH}^*} = 2.86 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 263–351 K (relative rate method, DeMore & Bayes 1999)

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

Half-Lives in the Environment:
Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); calculated lifetimes of 4.1 d and 180 d for reactions with OH radical, NO₃ radical, respectively (Atkinson 2000)

### TABLE 10.1.1.1.1
Reported vapor pressures of dimethyl ether at various temperatures and the coefficients for the vapor pressure equations

| t/°C | P/Pa | eq. 1 log P = A – B/(T/K) | ln P = A – B/(T/K) | eq. 2 log P = A – B/(C + t/°C) | ln P = A – B/(C + t/°C) | eq. 3 log P = A – B/(C + T/K) | ln P = A – B/(C + T/K) | eq. 4 log P = A – B/(C + log (T/K)) | ln P = A – B/(C + log (T/K)) | eq. 5 log P = A – B/(C + T/K) – C·log (T/K) | ln P = A – B/(C + T/K) – C·log (T/K) | eq. 6 log P = A – B/(T/K) + C·log (T/K) – D·(T/K) | ln P = A – B/(T/K) + C·log (T/K) – D·(T/K) |
|------|-----|--------------------------|-------------------|------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| −70.66 | 8121 | static method-manometer  | summary of literature data | static-pressure gauge       | quartz pressure sensors  | 233.128                  | 238.126                  | 243.157                  | 248.152                  | 253.152                  | 258.160                  | 263.160                  | 268.161                  |
| −65.25 | 11706 | 0.51                      | 270000             | 3.07                        | 300000                  | 4.97                     | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  |
| −60.03 | 16315 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −55.14 | 21910 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −49.90 | 29585 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −45.10 | 38334 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −40.02 | 49810 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −35.10 | 63401 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −27.67 | 89362 | −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |
| −24.91 | 100847| −93.3                     | 1333               | 4.97                        | 330000                  | 15.01                    | 430000                  | 20.50                    | 510000                  | 27.11                    | 630000                  | 27.11                    | 630000                  |

**mp/°C**
-141.5

**bp/°C**
-24.82

**Noles & Zollweg 1992**

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**temp range 195–284.34 K**

| A | 23.686185 |
| B | 1691.8056 |
| C | −6.04560 |
| D | 0.00195754 |
| temp range 195–284.34 K | 99.95 |

more to

| 400.378 | 535580 |
| 400.378 | 535580 |

data fitted to Wagner eq.
FIGURE 10.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl ether.
10.1.1.2 Diethyl ether (Ethyl ether)

Common Name: Diethyl ether
Synonym: ether, ethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane, sulfuric ether
Chemical Name: ether, diethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane
CAS Registry No: 60-29-7
Molecular Formula: C₄H₁₀O, CH₃CH₂OCH₂CH₃
Molecular Weight: 74.121
Melting Point (°C):
–116.2 (Lide 2003)
Boiling Point (°C):
34.5 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
0.7136, 0.7078 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
103.9 (20°C, calculated-density)
106.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
5.439 (quoted, Riddick et al. 1986)
7.19 (exptl., Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
60270* (thermostatic volumetric method, measured range –3.83 to 30°C, Hill 1923)
60400* (volumetric method, measured range 10–30°C, Kablukov & Malischeva 1925)
60300* (volumetric method, measured range 10–25°C, Bennett & Phillip 1928)
69000 (Seidell 1941; Lange 1971)
60400 (selected, Riddick et al. 1986)
60900 (literature data compilation, 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):
74690* (calculated-Antoine eq. regression, temp range –74 to 35.6°C, Stull 1947)
323835* (71.11°C, static method-Bourdon, measured range 71.11–187.78°C, Kobe et al. 1956)
$\log \left(\frac{P}{\text{mmHg}}\right) = \left[-0.2185 \times \frac{6946.2}{(T/\text{K})}\right] + 7.56659; \text{ temp range –74.3 to 183.3°C (Antoine eq., Weast 1972–73)}$
58920 (20°C, Verschueren 1983)
$\log \left(\frac{P}{\text{kPa}}\right) = 6.05115 – 1062.409/(T/\text{K}) – 44.967; \text{ temp range 250–329 K (ebulliometry, Antoine eq., Ambrose et al. 1972)}$
71620 (Ambrose et al. 1976)
71240, 71610 (calculated-Antoine eq., Boublik et al. 1984)
$\log \left(\frac{P}{\text{kPa}}\right) = 6.04972 – 1066.052/(220.003 + t/°C); \text{ temp range –70.0 to 19.87°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}$
$\log \left(\frac{P}{\text{kPa}}\right) = 6.0492 – 1061.391/(228.8 + t/°C); \text{ temp range –23.1 to 55.434°C (Antoine eq. from reported exptl. data of Ambrose et al. 1972, Boublik et al. 1984)}$
$\log \left(\frac{P}{\text{mmHg}}\right) = 6.92032 – 1064.07/(228.8 + t/°C); \text{ temp range –61 to 20°C (Antoine eq., Dean 1985, 1992)}$
71620 (selected, Riddick et al. 1986)
log (P/kPa) = 6.05115 – 1062.409/(228.183 + t/°C), temp range not specified ( Antoine eq., Riddick et al. 1986)
71620, 71604 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.02962 – 1051.432/(–44.967 + T/K); temp range 286–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.05115 – 1062.409/(–44.967 + T/K); temp range 250–329 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.05933 – 1067.576/(–44.217 + T/K); temp range 305–360 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.30714 – 1236.75/(–20.11 + T/K); temp range 307–457 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.37811 – 1276.822/(–14.869 + T/K); temp range 417–467 K (Antoine eq.-V, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m3/mol at 25°C or as indicated and reported temperature dependence):
130 (calculated-I/K_AW, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
90.0 (calculated-group contribution method, Hine & Mookerjee 1975)
237 (calculated-bond contribution method, Hine & Mookerjee 1975)
87.9 (calculated-P/C using Riddick et al. 1986 data)
86.8 (23°C, batch air stripping-IR, Nielsen et al. 1994)
95.05 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_AW = 5.953 – 2158/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_OW:
0.83 (20°C, shake flask-CR, Collander 1951)
1.03 (Hansch et al. 1968)
0.89 (shake flask-GC, both phases, Hansch et al. 1975)
0.77 (shake flask, Log P Database, Hansch & Leo 1987)
0.89 (recommended, Sangster 1989)
0.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_OA at 25°C:
2.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_OC:

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

Volatileization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_OH for reaction with OH radical, k_NO3 with NO3 radical and k_O3 with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_OH(calc) = 1.43 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_OH(observ.) = 1.34 × 10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_OH = 13.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 K, measured range 295–442 K (Tully & Droege 1987)
k_OH(exptl) = 1.34 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_OH(calc) = 1.06 × 10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_OH = (13.6 ± 0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)
k_OH = 1.36 × 10^{-11} cm^3 molecule^{-1} s^{-1}; k(soln) = 6.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988a)
k_OH = 1.20 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 294 K (relative rate method, Bennett & Keer 1989)
k_OH = 1.33 × 10^{-11} cm^3 molecule^{-1} s^{-1} 298 K (recommended, Atkinson 1989, 1990)
k_{OH} = (11.3 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by pulse radiolysis-UV spectroscopy; } k_{OH} = (12.8 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by relative rate method, at } 298 \pm 2 \text{ K (Nelson et al. 1990)}

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

Half-Lives in the Environment:
Air: disappearance t_{ds} < 0.24 h from the air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
calculated lifetimes of 11 h and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

**TABLE 10.1.1.2.1**
Reported aqueous solubilities of diethyl ether at various temperatures

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**FIGURE 10.1.1.2.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for diethyl ether.
### TABLE 10.1.1.2.2
Reported vapor pressures of diethyl ether 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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FIGURE 10.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl ether.
10.1.1.3 Methyl t-butyl ether (MTBE)

Common Name: Methyl t-butyl ether
Synonym: MTBE, 3-oxa-3,3-dimethylbutane, 2-methoxy-2-methyl-propane
Chemical Name: methyl tert-butyl ether
CAS Registry No: 1634-04-4
Molecular Formula: C₅H₁₂O, CH₃-O-C(CH₃)₃
Molecular Weight: 88.148
Melting Point (°C):
  −108.6 (Lide 2003)
Boiling Point (°C):
  55.0 (Lide 2003)
Density (g/cm³ at 20°C):
  0.7578 (Bennett & Phillip 1928)
  0.7404 (Windholz 1983; Budavari 1989)
Molar Volume (cm³/mol):
  119.1 (20°C, calculated-density)
  127.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘₑₙ (kJ/mol):
Entropy of Fusion, ∆Sₑₙ (J/mol K):
  7.60 (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  51600* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)
  48000 (Windholz 1983; Budavari 1989)
  52100 (literature data compilation, Yaws et al. 1990)
  42000* (19.8°C, shake flask-GC/TC, measured range 0–48.6°C, Stephenson 1992)
  62100, 35500 (5, 20°C, shake flask-GC, Fischer 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):
  log (P/kPa) = 6.09379 − 1173.036/(T/K) + 41.366; temp range 288–351 K (Antoine equation, comparative ebulliometry, Ambrose et al. 1976)
  32660 (Windholz 1983; Budavari 1989)
  33545 (calculated-Antoine eq., Stephenson & Malanowski 1987)
  log (P/kPa) = 6.09111 − 1171.54/(−41.542 + T/K); temp range 287–351 K (Antoine eq., Stephenson & Malanowski 1987)
  37417* (27.806°C, static method, measured range 301–411 K, Krähenbühl & Gmehling 1994)
  log (P/kPa) = 6.070343 − 1158.923/(T/K) − 43.20; temp range 301–411 K (Antoine eq., static method, Krähenbühl & Gmehling 1994)
  log (P/mmHg) = 4.7409 − 1.9493 × 10³/(T/K) + 3.077·log (T/K) − 1.4463 × 10⁻²·(T/K)²; temp range 165–497 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):
  59.46 (calculated as 1/Kₑₑₑₑₑₑ⁻¹, Cₖ/Cₐ, reported as exptl., Hine & Mookerjee 1975)
  142.6, 305 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)
  53.54*, 121 (25, 30°C, static headspace-GC, Robbins et al. 1993)
  63.2 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)
Octanol/Water Partition Coefficient, log $K_{ow}$:

1.06  (Hansch et al. 1968; Kier & Hall 1976)
1.30  (calculated-fragment const., Hansch & Leo 1979)
0.94  (shake flask-GC, Funasaki et al. 1985)
0.94  (recommended, Sangster 1989)
0.94  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

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

$k_{OH}$(calc) = $1.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}$(obs.) = $2.64 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}$(exptl) = $2.64 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}$(calc) = $1.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (3.09 \pm 0.15) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 3.09 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k$(soln) = $2.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 2.83 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = (2.44 - 3.09) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295–298 K (Atkinson 1989)

$k_{OH}^* = 2.98 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 293 K, measured range 293–750 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_1/2 < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnell et al. 1976);

calculated lifetimes of 3.9 d and 72 d for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000).
### TABLE 10.1.1.3.1
Reported aqueous solubilities of methyl tert-butyl ether (MTBE) at various temperatures

<table>
<thead>
<tr>
<th>Bennett &amp; Phillip 1928</th>
<th>Stephenson 1992</th>
<th>Fischer et al. 2004</th>
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<td><strong>shake flask-GC</strong></td>
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**FIGURE 10.1.1.3.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for methyl t-butyl ether (MTBE).
TABLE 10.1.1.3.2
Reported vapor pressures of methyl tert-butyl ether (MTBE) at various temperatures

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<th>t/°C</th>
<th>P/Pa</th>
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<th>P/Pa</th>
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<td>32.143</td>
<td>44576</td>
<td>log P = A – B/(C + t/°C)</td>
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**FIGURE 10.1.1.3.2** Logarithm of vapor pressure versus reciprocal temperature for methyl tert-butyl ether (MTBE).
### TABLE 10.1.1.3.3

Reported Henry’s law constants of methyl tert-butyl ether (MTBE) at various temperatures and temperature dependence equations

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

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<tr>
<th>Robbins 1993</th>
<th>Bierwagen &amp; Keller 2001</th>
<th>Fischer et al. 2004</th>
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<td><strong>t/°C</strong></td>
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<td>eq. 1</td>
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### FIGURE 10.1.1.3.3

Logarithm of Henry’s law constant versus reciprocal temperature for methyl t-butyl ether (MTBE).
10.1.1.4 Di-n-propyl ether

Common Name: Di-n-propyl ether
Synonym: 4-oxaheptane, 1,1′-oxibispropane, 1-propoxypropane, propyl ether
Chemical Name: di-n-propyl ether, propyl ether, 4-oxaheptane
CAS Registry No: 111-43-3
Molecular Formula: C₆H₁₄O, (n-C₃H₇)₂O
Molecular Weight: 102.174
Melting Point (°C): −114.8 (Lide 2003)
Boiling Point (°C): 90.08 (Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 20°C):
- 0.7466, 0.7419 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
- 136.9 (20°C, calculated-density)
- 151.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₜₚ (kJ/mol):
- 10.78 (quoted, Riddick et al. 1986)
Entropy of Fusion, ΔSₜₚ (J/mol K):
- Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
- 4900* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)
- 2500* (synthetic method, measured range 0–25°C, Bennett & Phillip 1928)
- 3000 (Séidell 1941; Lange 1971)
- 2508 (selected, Hine & Mookerjee 1975)
- 4900 (selected, Riddick et al. 1986)
- 3820 (literature data compilation, 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):
- 9072* (calculated-Antoine eq. regression, temp range −43.3 to 89.5°C, Stull 1947)
log (P/mmHg) = −0.2185 × 8229.6/(T/K) + 7.863332; temp range −43.3 to 89.5°C (Antoine eq., Weast 1972–73)
log (P/cmHg) = 5.894812 – 1227.468/(215.7007 + t°C); temp range 39.7–98.2°C (comparative ebulliometry, Meyer & Hotz 1973)
log (P/kPa) = 6.03075 – 123.148/{(T/K) + 56.708}; temp range 293–388 K (Antoine eq., ebulliometry, Ambrose et al. 1976)
- 8378, 8320 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.06887 – 1254.429/(218.781 + t°C); temp range 26.59–88.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.01902 – 1227.068/(215.654 + t°C); temp range 39.7–86.18°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9476 – 1256.5/(219.0 + t°C); temp range 26–89°C (Antoine eq., Dean 1985, 1992)
- 8334 (selected, Riddick et al. 1986)
log (P/kPa) = 6.03075 – 1133.748/(216.442 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
- 8334 (calculated-Antoine eq., Stephenson & Malanowski 1987)
Ethers

\[
\log (P_L/\text{kPa}) = 6.019715 - 1227.468/(–57.449 + T/\text{K}); \text{ temp range 312–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P_L/\text{kPa}) = 6.0361 - 1236.828/(–56.358 + T/\text{K}); \text{ temp range 292–389 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P_L/\text{kPa}) = 6.50879 - 1579.466/(–12.142 + T/\text{K}); \text{ temp range 385–467 K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]

\[
\log (P_L/\text{kPa}) = 8.20381 - 3494.323/(209.259 + T/\text{K}); \text{ temp range 465–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{mmHg}) = 44.0232 – 3.282 \times 10^3/(T/\text{K}) – 12.792 \cdot \log (T/\text{K}) + 1.2682 \times 10^{-10} \cdot (T/\text{K})^2; \text{ temp range 150–531 K (vapor pressure eq., Yaws 1994)}
\]

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

350.1 (calculated as 1/K_{AW}, C_W/C_A, reported as exp., Hine & Mookerjee 1975)
175.5, 594.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
223.3 (computer value, Yaws et al. 1991)

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

2.03 (shake flask, Hansch et al. 1968; Leo et al. 1971)
2.03 (recommended, Sangster 1989)
2.03 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

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

Volatilization:

Photolysis:

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

\[
k_{OH} = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K (relative rate, Lloyd et al. 1976)}
\]

\[
k_{OH}\text{(calc)} = 2.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}\text{(obs.)} = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)}
\]

\[
k_{OH}\text{(calc)} = 1.57 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}\text{(exptl)} = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1987)}
\]

\[
k_{OH}^* = (18.0 \pm 2.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)}
\]

\[
k_{OH} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 294 \pm 2 K (relative rate method, Bennett & Kerr 1989)}
\]

\[
k_{OH}^* = (19.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by pulse radiolysis-UV spectroscopy; k}_{OH} = (20.3 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by relative rate method, at 298 \pm 2 K (Nelson et al. 1990)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance t_1/2 < 0.24 h from air) for the reaction with OH radical (Darnall et al. 1976).
TABLE 10.1.1.4.1
Reported aqueous solubilities of di-n-propyl ether at various temperatures

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<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
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FIGURE 10.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-n-propyl ether.

TABLE 10.1.1.4.2
Reported vapor pressures of di-n-propyl ether at various temperatures and the coefficients for the vapor pressure equations

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summary of literature data comparative ebulliometry

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coefficients of Chebyshev eq. also given in text
10.1.1.5 Di-isopropyl ether

Common Name: Di-isopropyl ether
Synonym: diisopropoxyde, isopropyl ether, 2-isopropoxypropane, 2,2′-oxybispropane, 3-oxa-2,4-dimethylpentane, IPE, DIPE
Chemical Name: diisopropyl ether, isopropyl ether, 2-isopropoxypropane, 2,2′-oxybispropane, 3-oxa-2,4-dimethylpentane
CAS Registry No: 108-20-3
Molecular Formula: C₆H₁₄O, [(CH₃)₂CH]₂O
Molecular Weight: 102.174
Melting Point (°C):
-85.4 (Lide 2003)
Boiling Point (°C):
68.4 (Lide 2003)
Density (g/cm³ at 20°C):
0.7360 (Bennett & Phillip 1928)
0.7239, 0.7185 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
140.0 (20°C, calculated-density)
151.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
12.033 (quoted, Riddick et al. 1986)
12.05 (exptl., Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2040 (selected, Hine & Mookerjee 1975)
9000 (20°C, Verschueren 1983)
12000 (20°C, selected, Riddick et al. 1986)
11200 (literature data compilation, Yaws et al. 1990)
7900*, 5400 (20°C, 31°C, shake flask-GC/TC, measured range 0–61°C. Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
21410* (calculated-Antoine eq. regression, temp range –57 to 67.5°C, Stull 1947)
\[ \log (P/\text{mmHg}) = 7.09712 - 1257.6/(230 + t/°C) \] (Antoine eq., Dreisbach & Martin 1949)
20093* (temp range 0–60°C, Nicolini & Laffitte 1949)
21532* (26.8°C, ebulliometry, measured range 13.5–70.6°C, Flom et al. 1951)
\[ \log (P/\text{mmHg}) = [-0.2185 \times 7777.3/(T/K)] + 7.904664; \text{temp range } -57 \text{ to } 67.5°C \] (Antoine eq., Weast 1972–73)
\[ \log (P/\text{kPa}) = 5.97678 - 1143.073/(T/K) + 53.810; \text{temp range } 284–365 \text{ K} \] (Antoine eq., ebulliometry, Ambrose et al. 1976)
19954, 20120 (calculated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{kPa}) = 5.78384 - 1050.657/(209.511 + t/°C); \text{temp range } 0–60°C \] (Antoine eq. from reported exptl. data, Boublik et al. 1984)
\[ \log (P/\text{mmHg}) = 6.8495 - 1139.34/(218.7 + t/°C); \text{temp range } 23–67°C \] (Antoine eq., Dean 1985, 1992)
19880 (selected, Riddick et al. 1986)
log (P/kPa) = 5.97678 − 1143.073/(219.340 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
19950, 19890 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.966496 − 1135.034/(−54.92 + T/K); temp range 296–342 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.26597 − 1334.298/(80.78 + T/K); temp range 360–440 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 7.13537 − 2140.415/(80.78 + T/K); temp range 436–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
19862, 10850 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
log (P/mmHg) = 35.9552 − 2.0276 × 10³/(T/K) − 2.8551·log (T/K) + 2.7662 × 10⁻⁴·(T/K) − 9.9111 × 10⁻¹⁴·(T/K)²; temp range 188–500 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
1010 (calculated as 1/K AW, Cw/Cw, reported as expl., Hine & Mookerjee 1975)
483.3, 594.6 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)
175.6 (computer value, Yaws et al. 1991)
208.8 (23°C, batch air stripping-IR, Nielsen et al. 1994)
212.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
231 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, log K ow:
1.52 (shake flask-GC, Funasaki et al. 1985)
1.56 (calculated-fragment const., Hansch & Leo 1979)
1.52 (recommended, Sangster 1989)
1.52 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K oa:
2.66 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K oc:

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis: rate constant k, for gas-phase second order rate constants, k OH for reaction with OH radical, k NO3 with NO3 radical and k OW with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k OH = (1.07 ± 0.20) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy, k OH = (1.13 ± 0.20) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K by relative rate technique (Nelson et al. 1990)

k OH = (1.08 ± 0.09) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 296 K, measured range 240–400 K (absolute rate, flash photolysis-resonance fluoresence, Wallington et al. 1993)

k OH = (9.9 ± 0.2) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ and (1.07 ± 0.6 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Wallington et al.1993)

k OH = 9.8 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K using both relative (at 295 K) and absolute techniques over 240–440 K (FT-IR spectroscopy, Wallington et al. 1993)

k OH = 2.2 × 10⁻¹² exp[(445 ± 1450)/(T/K)]; temp range 240–440 K (Arrhenius eq., FT-IR, Wallington et al. 1993)

k OH(calc) = 33.3 × 10⁻¹² cm³ mol⁻¹ s⁻¹, k OH(exptl) = 10.2 × 10⁻¹² cm³ mol⁻¹ s⁻¹ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

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

Half-Lives in the Environment:
Air: disappearance \(t_{50} < 0.24\) h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

<table>
<thead>
<tr>
<th>TABLE 10.1.5.1</th>
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<tr>
<td>Reported aqueous solubilities of di-isopropyl ether at various temperatures</td>
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**FIGURE 10.1.5.1** Logarithm of mole fraction solubility \((\ln x)\) versus reciprocal temperature for di-isopropyl ether.
### TABLE 10.1.5.2

Reported vapor pressures of di-isopropyl ether at various temperatures and the coefficients for the vapor pressure equations

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

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<th>t/°C</th>
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**Stull 1947**

**Nicolini & Laffitte 1949**

**Cidlinsky & Polak 1969 in Boublík et al. 1984**

**Ambrose et al. 1976 comparative ebulliometry**

**Flom et al. 1951 dynamic-ebulliometry**

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Coefficients of Chebyshev also given in text.
FIGURE 10.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for di-isopropyl ether.
10.1.1.6 Butyl ethyl ether

Common Name: Butyl ethyl ether
Synonym: butyl ethyl ether, 1-ethoxybutane, n-butyylethyl ether, 3-oxaheptane
Chemical Name: butylethyl ether, 1-ethoxybutane, n-butyylethyl ether
CAS Registry No: 628-81-9
Molecular Formula: C₆H₁₄O, C₄H₉OCH₂CH₃
Molecular Weight: 102.174
Melting Point (°C):
-124 (Lide 2003)
Boiling Point (°C):
92.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.7495, 0.7448 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
136.3 (20°C, calculated-density)
150.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, 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):
6500* (20°C, shake flask-GC/TC, measured range 0–90.7°C, Stephenson 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):
303164* (126.67°C, static-Bourdon gauge, measured range 126.67–237.78°C, Kobe et al. 1956)
13912* (38.18°C, ebulliometry, measured range 38.18–91.38°C, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)
log (P/kPa) = 6.06257 – 1252.485/{(T/K) + 56.685} (Antoine eq., Ambrose et al. 1976)
9090 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.06565 – 1234.258/{226.668 + t/°C}; temp range 38.18–91.38°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.9444 – 2.4667 × 10⁻³/{216.9 + t/°C}; temp range 38–92°C (Antoine eq., Dean 1985, 1992)
7461 (quoted, Riddick et al. 1986)
log (P/kPa) = 6.06257 – 1252.485/{216.465 + t/°C}, temp range not specified (Antoine eq., Riddick et al. 1986)
7510 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.062575 – 1252.485/{–56.685 + T/K}; temp range 311–365 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 8.5224 – 2.4667 × 10⁻³/(T/K) + 1.0513·log (T/K) – 1.4047 × 10⁻²·(T/K) + 9.2664 × 10⁻⁶·(T/K)²; temp range 170–531 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
136 (calculated-P/C from selected data)
241 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)
Octanol/Water Partition Coefficient, log K_ow:
2.03 (shake flask-GC, Hansch & Anderson 1967)
2.03 (recommended, Sangster 1989)
2.03 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

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

$k_{OH} = 2.28 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.34 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294 ± 2 K (relative rate, Bennett & Kerr 1989)

$k_{OH} = (13.4 - 22.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294–298 K (review, Atkinson 1989)

$k_{OH} = (18.7 \pm 0.7) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (pulse radiolysis-UV spectroscopy, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance $t_{0.5} < 0.24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

<table>
<thead>
<tr>
<th>TABLE 10.1.1.6.1</th>
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<tbody>
<tr>
<td>Reported aqueous solubilities of butyl ethyl ether at various temperatures</td>
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<td>Stephenson 1992</td>
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FIGURE 10.1.1.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for butyl ethyl ether.

TABLE 10.1.1.6.2
Reported vapor pressures of butyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

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Kobe et al. 1956 static-Bourdon gauge

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Cidlinsky & Polak 1969 in Boublik et al. 1984

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<th>Pressure $P$ $A/B/(T/K)$</th>
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FIGURE 10.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for butyl ethyl ether.
10.1.1.7  Di-n-butyl ether

Common Name: Di-n-butyl ether
Synonym: 1-butoxybutane, butyl ether, dibutyl ether, n-butyl ether, 5-oxanonane, 1,1′-oxybisbutane
Chemical Name: butyl ether, dibutyl ether, di-n-butyl ether, n-butyl ether, 5-oxanonane, 1,1′-oxybisbutane
CAS Registry No: 142-96-1
Molecular Formula: C₈H₁₈O, (n-C₄H₉)₂O
Molecular Weight: 130.228
Melting Point (°C):
-95.2  (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
140.28  (Lide 2003)
Density (g/cm³ at 20°C):
0.76889, 0.76461 (20°C, 25°C, Dreisbach & Martin 1949)
0.7684, 0.7641 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
170.0  (calculated-density, Wang et al. 1992)
196.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C, 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):
< 100  (17°C, synthetic method, Bennett & Phillip 1928)
300  (20°C, Verschueren 1983; Riddick et al. 1986)
230*  (19.9°C, shake flask-GC/TC, measured range 0–90.6°C, Stephenson 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):
7605*  (66.84°C, ebulliometry, measured range 67–142°C, Dreisbach & Shrader 1949)
log (P/mmHg) = 7.31540 – 1648.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
80612*  (237.78°C, static method-Bourdon gauge, measured range 238–293°C, Kobe et al. 1956)
19529*  (89.14°C, ebulliometry, measured range 89.14–140°C, Cidlinsky & Polak 1969)
log (P/kPa) = 5.93018 – 1302.768/(T/K– 81/481); temp range 89–140°C (Cidlinsky & Polak 1969)
log (P/kPa) = 5.93018 – 1302.768/{(T/K) – 81.481} (Antoine eq., ebulliometry, Ambrose et al. 1976)
640  (20°C, Verschueren 1983)
825, 874  (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.151 – 1458.718/(141.982 + t/°C); temp range 66.8–141.97°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.92274 – 1298.256/(191.144 + t/°C); temp range 89.14–140.06°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.7963 – 1297.3/(191.03 + t/°C); temp range 89–140°C (Antoine eq., Dean 1985, 1992)
898  (select, Riddick et al. 1986)
log (P/kPa) = 5.930185 – 1302.768/(191.669 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 6.4403 – 1648.4/(-42.15 + T/K); temp range 339–415 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/mmHg) = 12.9321 – 3.0416 × 10⁷/(T/K) + 0.42929·log (T/K) – 1.237 × 10⁻²·(T/K) + 7.5943 × 10⁻⁶·(T/K)²; temp range 178–581 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
608.5 (calculated-1/K₃₉W, C₇/W/C₇, reported as exptl., Hine & Mookerjee 1975)
350, 1362 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log Kₙ₉₉₉:
3.08 (calculated-f const., Hansch & Leo 1979)
3.21 (shake flask-GC, Funasaki et al. 1984)
3.21 (recommended, Sangster 1989)
3.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₙ₉₉₉:
3.89 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Kₙ₉₉₉:

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k₉₉₉ for reaction with OH radical, k₉₉₉ with NO₃ radical and k₉₉₉ with O₃ or as indicated, *data at other temperatures see reference:
k₉₉₉ = (27.8 ± 3.6) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)
k₉₉₉ = 17 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)
k₉₉₉ = (17.0 – 27.8) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294–298 K (review, Atkinson 1989)
k₉₉₉ = (27.2 ± 0.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy; k₉₉₉ = (28.8 ± 1.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

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

Half-Lives in the Environment:
Air: disappearance t₉₉₉ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

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<th>t/°C</th>
<th>S/g·m⁻³</th>
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TABLE 10.1.1.7.1
Reported aqueous solubilities of di-n-butyl ether at various temperatures

Stephenson 1992

shake flask-GC/TC
**TABLE 10.1.1.7.2**

Reported vapor pressures of di-\textit{n}-butyl ether at various temperatures and the coefficients for the vapor pressure equations

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

---

<table>
<thead>
<tr>
<th>Dreisbach &amp; Shrader 1949</th>
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**FIGURE 10.1.1.7.1** Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for di-\textit{n}-butyl ether.
FIGURE 10.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for di-\( \text{n} \)-butyl ether.
10.1.1.8 1,2-Propylene oxide

Common Name: 1,2-Propylene oxide
Synonym: 1,2-epoxypropane, methyloxirane, propylene oxide
Chemical Name: 1,2-propylene oxide, 1,2-epoxypropane, propylene oxide
CAS Registry No: 75-56-9
Molecular Formula: C₃H₆O
Molecular Weight: 58.079
Melting Point (°C):
-111.9 (Lide 2003)
Boiling Point (°C):
35 (Lide 2003)
Density (g/cm³ at 20°C):
0.859 (0°C, Verschueren 1983)
Molar Volume (cm³/mol):
69.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{ fus} (kJ/mol):
6.57, 6.53 (exptl., Chickos et al. 1999)
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 or as indicated):
476000 (US EPA 1981; quoted, Howard 1989)
405000, 650000 (20°C, 30°C, Verschueren 1983)
259000 (literature data compilation, Yaws et al. 1990)
139320 (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):
74520* (calculated-Antoine eq., regression, temp range –75 to 34.5°C, Stull 1947)
530538* (87.78°C, static method, measured range 88–204°C, Kobe et al. 1956)
51969* (17.05°C, ebulliometry, measured range –24.17 to 34.75°C (McDonald et al. 1959)
log (P/mmHg) = 6.96997 – 1065.27/(226.283 + t/°C); temp range –24.17 to 34.75°C (ebulliometry, McDonald et al. 1959)
70112* (interpolated-Antoine eq., static method, measured range 19.0–71.8°C Bott & Sadler 1966)
log (P/mmHg) = 7.658 – 1472/(T/K); temp range 19.0–71.8°C (Antoine eq., static method, Bott & Sadler 1966)
log (P/mmHg) = [–0.2185 × 7295.8/(T/K)] + 8.093473; temp range –75 to 34.5°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = 7.06492 – 1113.6/(232.0 + t/°C); temp range –35 to 130°C (Antoine eq., Dean 1985, 1992)
59300, 75900 (20, 25°C, Riddick et al. 1986)
log (P/kPa) = 6.09487 – 1065.27/(226.283 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
71700 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.09487 – 1065.27/(-46.867 + T/K); temp range 225–308 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 38.5381 – 2.631 × 10^5/(T/K) – 11.104-log (T/K) + 4.2178 × 10^-10 × (T/K) + 5.5025 × 10^-6 × (T/K)^2; temp range 161–482 K (vapor pressure eq., Yaws 1994)
log (P/kPa) = 4.05984 + 1086.37/[(T/K) – 44.4556]; temp range not specified (Antoine eq., Horstmann et al. 2004)
Henry’s Law Constant (Pa m³/mol at 25°C):
8.653 (calculated-P/C, Howard 1989)
Octanol/Water Partition Coefficient, log K_{ ow}:
0.03 (shake flask, Hansch & Leo 1985, 1987)

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Bioconcentration Factor, log BCF:
−0.20, −0.40 (calculated, Howard 1989)

Sorption Partition Coefficient, log KOC:
0.623 (estimated-S, Lyman et al. 1982; quoted, Howard 1989)
1.477 (calculated-QSAR, Sabljic 1984; quoted, Howard 1989)

Environmental Fate Rate Constants, k, and Half-Lives:
Volatilization: t½(calc) ~ 3 and 18 d from a representative or natural river and oligotrophic lake, respectively
(USEPA 1986; quoted, Howard 1989).

Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:
kOH(exptl) = 5.2 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, kOH(calc) = 4.5 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for gas phase reactions;

k = 2.4 × 10⁸ cm³ mol⁻¹ s⁻¹ for the reaction with photochemically produced OH radical in water at room temp. (Güesten et al. 1981; quoted, Howard 1989)

photooxidation t½ = 19.3 d can be calculated for the gas phase reaction with OH radical in air by using
Güesten 1981 data and assuming an average OH radical concn. of 8 × 10⁹ molecules/cm³ (GEMS 1986; quoted, Howard 1989)

kOH = (1.11 ± 0.75) × 10⁻¹² cm³ molecule⁻¹·s⁻¹ with reference to n-butane for the gas phase reaction with
OH radical in air at (23.1 ± 1.1)°C with an atmospheric lifetime of 10 d for an average concentration of
1 × 10⁹ molecules/cm³ of OH radical (Edney et al. 1986)

kOH(calc) = 5.4 × 10⁻¹³ cm³ molecule⁻¹·s⁻¹; kOH(exptl) = 5.2 × 10⁻¹³ cm³ molecule⁻¹·s⁻¹ at room temp. (SAR,
Atkinson 1987)

kOH = (4.95 ± 0.52) × 10⁻¹³ cm³ molecule⁻¹·s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

kOH = 4.95 × 10⁻¹³ cm³ molecule⁻¹·s⁻¹; k(soln) = 4.2 × 10⁻¹³ cm³ molecule⁻¹·s⁻¹ for reaction with OH radical
in aqueous solution (Wallington et al. 1988b)

Hydrolysis: estimated t½ ~ 11.6 d in fresh water at pH 7 to 9 and t½ = 6.6 d at pH 5 (Howard 1989).

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

Half-Lives in the Environment:
Air: disappearance t½ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

atmospheric lifetime of 10 d (Edney et al. 1986);

Surface water: calculated t½ = 9.15 yr in natural water by using Güesten et al. 1981 data and assuming
an average OH radical concn. of 8 × 10⁹ molecules/cm³ (GEMS 1986; quoted, Howard 1989).

Surface water: calculated t½ = 9.15 yr in natural water by using Güesten et al. 1981 data and assuming an average
OH radical concentration of 1 × 10⁻¹⁷ M in natural water (Howard 1989).

Surface water:

Ground water:

Sediment:

Soil:

Biota:
TABLE 10.1.1.8.1
Reported vapor pressures of 1,2-propylene oxide at various temperatures and the coefficients for the vapor pressure equations

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

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<tr>
<th>Summary of lit. data</th>
<th>Kobe et al. 1956</th>
<th>McDonald et al. 1959</th>
<th>Bott &amp; Sadler 1966</th>
</tr>
</thead>
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<td>P/Pa</td>
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FIGURE 10.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-propylene oxide.

1,2-Propylene oxide: vapor pressure vs. 1/T

- Kobe et al. 1956
- McDonald et al. 1959
- Bott & Sadler 1966
- Stull 1947

b.p. = 35 °C
m.p. = -111.9 °C
10.1.1.9 Furan

Common Name: Furan
Synonym: 1,4-epoxy-1,3-butadiene, divinylene oxide, furfuran, oxole, tetrole
Chemical Name: 1,4-epoxy-1,3-butadiene, divinylene oxide, furan
CAS Registry No: 110-00-9
Molecular Formula: C₄H₄O
Molecular Weight: 68.074
Melting Point (°C):
-85.61 (Lide 2003)
Boiling Point (°C):
31.5 (Lide 2003)
Density (g/cm³ at 20°C):
0.9378 (Dreisbach 1955; Riddick et al. 1986)
0.9514 (Weast 1982–83)
Molar Volume (cm³/mol):
72.6 (20°C, calculated-density)
73.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
3.803 (Riddick et al. 1986)
2.05, 3.80 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
10070 (literature average, Valvani et al. 1981)
10000 (Verschueren 1983)
10000 (Riddick et al. 1986)
9900 (literature data compilation, Yaws et al. 1990)
26500 (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):
70109* (21.614°C, comparative ebulliometry, measured range 2.552–61.43°C, Guthrie et al. 1952)
\log (P/\text{mmHg}) = 6.97523 - 1060.851/(t/°C + 227.740); temp range 2.5–61.43°C (Antoine eq., comparative ebulliometry, Guthrie et al. 1952)
79980 (calculated from determined data, Dreisbach 1955)
\log (P/\text{mmHg}) = 6.97523 - 1060.851/(t/°C + 227.740); temp range –35 to 90°C (Antoine eq. for liquid state, Dreisbach 1955)
627000* (93.33°C, static-Bourdon gauge, measured range 93.33–210°C, Kobe et al. 1956)
\log (P/\text{mmHg}) = \left[1 – 304.367/(T/K]\right] \times 10^{8.58337 – 8.56435 \times 10^{-4}(T/K) + 9.32123 \times 10^{-7}(T/K)^2}; temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)
70110 (21.61°C, quoted, Boublik et al. 1984)
79930 (calculated-Antoine eq., Boublík et al. 1984)
\log (P/\text{kPa}) = 6.10017 – 1060.871/(227.742 + t/°C); temp range: 2.552–61.43°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
\log (P/\text{mmHg}) = 6.97527 – 1060.872/(227.74 + t/°C); temp range: 2–61°C (Antoine eq., Dean 1985, 1992)
84530 (selected, Riddick et al. 1986)
\log (P/\text{kPa}) = 6.10013 – 1060.851/(227.74 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
79930 (calculated-Antoine eq., Stephenson & Malanowski 1987)
\log (P/\text{kPa}) = 6.10013 – 1060.851/(-45.41 + T/K); temp range 238–363 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 24.9555 – 2.1624 × 10^3/(T/K) – 6.1066·log (T/K) – 2.4185 × 10–10·(T/K)²;  
temp range 188–490 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
575.5  (calculated-P/C using Riddick et al. 1986 data)
545.8  (computed-vapor liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log Kₐw:
1.34  (Hansch & Leo 1979;)
1.13  (estimated-HPLC, Garst 1984)
1.14, 1.35  (estimated-MO, π substituent consts., Bodor et al. 1989)
1.34  (recommended, Sangster 1989)
1.34  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Kₐc:
1.50, 1.46; 1.48  (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

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

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO₃ with NO₃ radical and kO₃ with O₃; or as indicated, *data at other temperatures and/or the Arrhenius expression
see reference:
k = 1.4 × 10¹⁰ M⁻¹ s⁻¹ oxidation rate by singlet oxygen in water (Mill 1980; quoted, Mill & Mabey 1985)
kOH = (4.01 ± 0.30) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ with a atmospheric lifetime τ ~ 7 h, kO₃ = (2.42 ± 0.28) × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K; and kO₃/T³ ~ 1.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with O³(P) atom at 298 K (relative rate method, Atkinson et al. 1983)
kOH = (3.98 ± 0.35) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 22 ± 2°C (relative rate method, Tuazon et al. 1984)
kOH = (40.8, 43.1) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 297 K, measured range 254–424 K (FP-RF flash photolysis-resonance fluorescence, Wine & Thompson 1984)
kO₃ = 2.4 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.15 d⁻¹, kOH = 4.0 × 10⁻¹ cm³ molecule⁻¹ s⁻¹ with a loss rate of 3.5 d⁻¹, and kNO₃ = 1.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a loss rate of 29 d⁻¹ at room temp. (review, Atkinson & Carter 1984)
kO₃ = 2.4 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.15 d⁻¹, kOH = 4.0 × 10⁻¹ cm³ molecule⁻¹ s⁻¹ with a loss rate of 1.7 d⁻¹, and kNO₃ = 1.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a loss rate of 29 d⁻¹ at room temp. (review, Atkinson 1985)
kNO₃ = (1.4 ± 0.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 295 ± 2 K (relative rate method, Atkinson et al. 1985)
kO₃ = 2.4 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ with a calculated tropospheric lifetime τ = 6.7 d, kOH = 4.0 × 10⁻¹ cm³ molecule⁻¹ s⁻¹ with a calculated τ = 50 min at room temp. (Atkinson et al. 1985)
kOH = 4.07 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ (Atkinson 1987, 1988; quoted, Müller & Klein 1991)
kOH = 4.046 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, kNO₃ = 1.439 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 295 K (Atkinson 1986 and Atkinson et al. 1988, Sabljic & Güsten 1990; Atkinson 1991)
kNO₃ = 1.44 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)
kOH = 4.05 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:
Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); calculated atmospheric lifetimes: 6.7 d due to reaction with O$_3$ in 24-h, 6.9 h due to reaction with OH radical in daytime and 50 min with NO$_3$ radical at room temp. (Atkinson et al. 1985).

Surface water: $t_{1/2} = 1.0$ h, estimated from oxidation rate by singlet oxygen of $1.4 \times 10^8$ M$^{-1}$ s$^{-1}$ (Mill 1980; quoted, Mill & Mabey 1985).

Ground water:

Sediment:

Soil:

Biota:

---

### TABLE 10.1.9.1

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

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<th>Temperature ($t/°C$)</th>
<th>Comparative ebulliometry</th>
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<td>21.614</td>
<td>70109</td>
<td>$\Delta H_f/(\text{kJ mol}^{-1}) = 27.09$</td>
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<td>84525</td>
<td>at bp</td>
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**FIGURE 10.1.1.9.1** Logarithm of vapor pressure versus reciprocal temperature for furan.
10.1.1.10  2-Methylfuran

Common Name: 2-Methylfuran
Synonym: silvan, sylvan
Chemical Name: 2-methylfuran
CAS Registry No: 534-22-5
Molecular Formula: C₅H₆O
Molecular Weight: 82.101
Melting Point (°C):
   −91.3  (Lide 2003)
Boiling Point (°C):
   64.7  (Lide 2003)
Density (g/cm³ at 20°C):
   0.913  (Verschueren 1983)
Molar Volume (cm³/mol):
   89.9  (20°C, calculated-density)
   95.7  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
   8.66 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₘₚ (J/mol K):
   4.97 (calculated-Le Bas method at normal boiling point)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   3000  (20°C, Verschueren 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):
   358285*  (110°C, static-Bourdon gauge, measured range 110–254.44°C, Kobe et al. 1956)
   86126*  (60.3°C, isoteniscop/manometry, measured range 60.3–100.3°C, Eon et al. 1971)
   log (P/mmHg) = [1– 338.704/(T/K)] × 10^(0.871223 – 7.95690 × 10^-1·(T/K) + 7.81737 × 10^-7·(T/K)^2); temp range 333.45–527.61 K (Cox eq., Chao et al. 1983)
   18930, 29990 (20°C, 30°C, quoted, Verschueren 1983)
   23090 (calculated-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 6.81244 − 1641.052/(276.164 + t°C); temp range 60.3–100.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   23250 (calculated-Antoine eq., Stephenson & Malanowski 1987)
   log (P/kPa) = 5.9.55585 − 1107.3/(−56.88 + T/K); temp range 251–338 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
   518  (20°C, calculated-P/C using Verschueren 1983 data)
Octanol/Water Partition Coefficient, log Kₐw:
   1.85 (shake flask, Log P Database, Hansch & Leo 1987)
   1.85 (recommended, Sangster 1989)
   1.85 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:
Air: disappearance $t_\frac{1}{2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

### TABLE 10.1.1.10.1
Reported vapor pressures of 2-methylfuran at various temperatures and the coefficients for the vapor pressure equations

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<th>P/Pa</th>
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Kobe et al. 1956

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Eon et al. 1971

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$\Delta H_v/(kJ \ mol^{-1}) = 30.79$

**FIGURE 10.1.1.10.1** Logarithm of vapor pressure versus reciprocal temperature for methylfuran.
10.1.1.11 Tetrahydrofuran

Common Name: Tetrahydrofuran
Synonym: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetramethylene oxide
Chemical Name: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetrahydrofuran, tetramethylene oxide
CAS Registry No: 109-99-9
Molecular Formula: C₄H₈O
Molecular Weight: 72.106
Melting Point (°C):
\[ -108.44 \] (Lide 2003)
Boiling Point (°C):
\[ 65 \] (Lide 2003)
Density (g/cm³ at 20°C):
\[ 0.8880 \] (Verschueren 1983)
\[ 0.8892 \] (Riddick et al. 1986)
Molar Volume (cm³/mol):
\[ 81.1 \] (20°C, calculated-density)
\[ 88.3 \] (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
\[ 8.535 \] (quoted, Riddick et al. 1986)
\[ 8.54 \] (exptl., Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Verschueren 1983; 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):
\[ 23465^* \] (dynamic-ebulliometry, measured 15–65°C, Flom et al. 1951)
\[ 434076^* \] (121.11°C, static-Bourdon gauge, measured range 121.11–265.56°C, Kobe et al. 1956)
\[ 19920^* \] (23.139°C, measured range 23.2–99.7°C, Scott et al. 1970)
\[ 21646^* \] (measured range 0.35–35°C, Koizumi & Ouchi 1970; quoted, Boublik et al. 1984)
\[ \log (P/\text{mmHg}) = [1– 339.244/(T/K)] \times 10^{0.830424 – 6.81525 \times 10^{-4}·(T/K) + 6.84786 \times 10^{-7}·(T/K)^2}; \text{ temp range 253.15–540.15 K (Cox eq., Chao et al. 1983)} \]
\[ 17530, 26340 \] (20°C, 30°C, quoted, Verschueren 1983)
\[ 21610, 21630 \] (calculated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{kPa}) = 6.59372 – 1446.15/(249.982 + t/°C); \text{ temp range 0.35–35°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]
\[ \log (P/\text{kPa}) = 6.12023 – 1202.394/(226.267 + t/°C); \text{ temp range 23.139–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]
\[ \log (P/\text{mmHg}) = 6.97231 – 540.5/(260.10 + t/°C); \text{ temp range not specified (Antoine eq., Dean 1985, 1992)} \]
\[ 19920, 21600, 26870 \] (23.139, 25, 30°C, Riddick et al. 1986)
\[ \log (P/\text{kPa}) = 6.79696 – 1157.06/(t/°C + 206.75), \text{ temp range: 90–140°C, (Antoine eq., Riddick et al. 1986)} \]
\[ 21620, 21900 \] (calculated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{mmHg}) = 5.92617 – 1101.47/(–57/95 + T/K); \text{ temp range 273–339 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 6.12052 – 1626.656/(15.041 + T/K); \text{ temp range 399–479 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 6.12052 – 1626.656/(15.041 + T/K); \text{ temp range 399–479 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

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log (P/kPa) = 6.73137 – 1702.922/(23.613 + T/K); temp range 467–541 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = 34.870 – 2.7523 × 10³/(T/K) – 9.5958·log (T/K) + 1.9889 × 10⁻¹⁰·(T/K)²; temp range 165–540 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
7.15 (calculated-I/K₆W, C₆W/C₆, reported as exptl., Hine & Mookerjee 1975)
10.33, 142.6 (calculated-group contribution calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol Water Partition Coefficient, log K₆W:
0.46 (calculated-f const., Hansch & Leo 1979)
0.22 (shake flask-GC, Funasaki et al. 1985)
0.46 (shake flask, Log P Database, Hansch & Leo 1987)
0.46 (recommended, Sangster 1989)
0.46 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K₆A:
2.86 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K₆S:
1.37, 1.26; 1.33 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

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

Volatilization:
Photolysis:
Oxidation: first 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 = (1.59 – 1.63) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (FP-RF flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)
kOH(calc) = 1.66 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, kOH(obs.) = 1.5 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)
kOH(exptl) = 1.50 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, kOH(calc) = 1.28 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1986, 1987; quoted, Sabljic & Güsten 1990)
kOH(calc) = 1.28 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987, 1988; quoted, Müller & Klein 1991)
kNO₃(calc) = 4.875 × 10⁻¹⁵ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Atkinson 1991)
kNO₃(calc) = 4.88 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)
kOH(calc) = 1.78 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 296 K (RP-RF method, Wallington et al. 1988b)
kOH(calc) = 1.61 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)
kOH(calc) = 18.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by relative rate method; kOH(calc) = 16.7 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 16 h at 298 ± 2 K; measured range 263–372 K (Moriarty et al. 2003)

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

Half-Lives in the Environment:
Air: disappearance t½ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
Surface water:
Ground water:
Sediment:
Soil: disappearance $t_{1/2} = 5.7$ d was calculated from measured first-order rate constant (Anderson et al. 1991).

Biota:

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**FIGURE 10.1.11.1** Logarithm of vapor pressure versus reciprocal temperature for tetrahydrofuran.
10.1.1.12 Tetrahydropyran

Common Name: Tetrahydropyran
Synonym: pentamethylene oxide, oxacyclohexane
Chemical Name: 1,5-epoxypentane, pentamethylene oxide, oxacyclohexane, tetrahydro-2H-pyran
CAS Registry No: 142-68-7
Molecular Formula: C₅H₁₀O
Molecular Weight: 86.132
Melting Point (°C):
  -49.1  (Lide 2003)
Boiling Point (°C):
  88.0  (Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
  0.8814, 0.8772 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  97.7  (20°C, calculated-density)
  107.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, 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):
  80200  (selected, Riddick et al. 1986)
  85700*, 68800 (19.9°C, 31°C, shake flask-GC/TC, measured range 0–81.3°C, Stephenson 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  9536  (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  log (P_L/kPa) = 6.01171 – 1249.062/(–49.943 + T/K; temp range 273–362 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
  12.71  (calculated-1/K_AW, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)
  13.94, 215.9 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
Octanol/Water Partition Coefficient, log K_ow:
  0.64  (shake flask-GC, Funasaki et al. 1985)
  0.82  (recommended, Sangster 1989)
  1.00  (recommended, Sangster 1993)
  0.95  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_oa:
  3.22  (head-space GC, Abraham et al. 2001)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_OC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_OH for reaction with OH radical, k_NO3 with NO3 radical and k_O3 with O3 or as indicated, *data at other temperatures see reference:
kOH $\sim 13.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989) 
kOH$^*$ = $11.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by relative rate method; kOH = $12.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 28 h at 298 ± 2 K, measured range 263–372 K (Moriarty et al. 2003).

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

Half-Lives in the Environment:
Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976); photodecomposition $t_{1/2} = 3.4$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976).

### TABLE 10.1.1.12.1
Reported aqueous solubilities of tetrahydropyran at various temperatures

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**FIGURE 10.1.1.12.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tetrahydropyran.
10.1.1.13 1,4-Dioxane

Common Name: 1,4-Dioxane
Synonym: 1,4-diethylenedioxy, glycoethyleneether,  p-dioxane
Chemical Name: 1,4-dioxane
CAS Registry No: 123-91-1
Molecular Formula: C₄H₈O₂
Molecular Weight: 88.106
Melting Point (°C):
11.85  (Lide 2003)
Boiling Point (°C):
101.5  (Lide 2003)
Density (g/cm³ at 20°C):
1.03318, 1.02766 (20°C, 25°C, Hovorka et al. 1936)
1.0336, 1.0280 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
85.2  (20°C, calculated-density)
92.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
12.46  (quoted, Riddick et al. 1986)
12.84  (exptl., Chickos et al. 1999)
Entropy of Fusion, ∆S_fus (J/mol K):
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Verschueren 1983; Riddick et al. 1986; Howard 1990)
miscible (Yaws et al. 1990)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations, *data at other temperatures are tabulated at end of this section):
4920* (static method, measured range 10–80°C, Hovorka et al. 1936)
log (P/mmHg) = 8.0588 – 1933.8/(T/K); temp range 10–80°C (Antoine eq., static method, Hovorka et al. 1936)
log (P/mmHg) = 7.8642 – 1866.7/(T/K); temp range ~ 10–110°C (Antoine eq., differential manometer, Gallaugher & Hibbert 1937)
4986* (static-Hg manometer, measured range 20–105°C, Crenshaw et al. 1938; quoted, Vinson & Martin 1963)
log (P/mmHg) = –2316.26/(T/K) – 2.77251·log (T/K) + 16.2007; temp range 20–105°C (Hg manometer, Crenshaw et al. 1938)
5333* (summary of literature data, Stull 1947)
406516* (154.44°C, static-Bourdon gauge, measured range 154.44–310°C, Kobe et al. 1956)
log (P/mmHg) = [-0.2185 × 8546.2/(T/K)] + 7.864110; temp range –35.8 to 101°C (Antoine eq., isomer not specified, Weast 1972–73)
5065  (Boublik et al. 1984)
4932  (quoted, Verschueren 1983)
log (P/kPa) = 6.66014 – 1556.983/(240.366 + t°C); temp range 20–105°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.56891 – 1550.445/(240.459 + t°C); temp range 20–125°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
4950, 6135 (25, 30°C, Riddick et al. 1986)
log (P/kPa) = 6.9891 – 1866.7/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
4915  (calculated-Antoine eq., Stephenson & Malanowski 1987)
log \( \frac{P}{kPa} = 6.40318 - 1457.97/(T/K) \); temp range 285–375 K (Antoine eq., Stephenson & Malanowski 1987)

5060, 6092 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

\[
\log (P/mmHg) = 20.5761 - 2.4658 \times 10^{-3}/(T/K) - 4.3645 \times 10^{-6}/(T/K)^2; \text{ temp range 285–587 K (vapor pressure eq., Yaws 1994)}
\]

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

0.495 (calculated as 1/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1990)

0.431, 1.564 (calculated-group contribution, calculated-bond contribution method Hine & Mookerjee 1975)

0.698 (computer value, Yaws et al. 1991)

1.609, 4.314, 6.925, 10.19 (dioxane, 40, 60, 70, 80°C, equilibrium headspace-GC, Kolb et al. 1992)

\[
\ln \left( \frac{1}{K_{AW}} \right) = -7.940 + 4798/(T/K), \text{ temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)}
\]

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

\[-0.42, 0.01 \] (observed, calculated-f const., Chou & Jurs 1979)

\[-0.42 \] (quoted, Verschueren 1983; quoted, Pinal et al. 1990)

\[-0.27 \] (Hansch & Leo 1985; quoted, Howard 1990; Capel & Larson 1995)

\[-0.27 \] (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log \( BCF \):

1.23 (soil, estimated-K_{OW}, Lyman et al. 1982)

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

Volatilization: estimated Henry’s law constant suggests that volatilization for 1,4-dioxane from water and moist soil should be slow; however, it has a moderate vapor pressure, so volatilization from dry soil is possible (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 as indicated, *data at other temperatures see reference:

photooxidation \( t_{\frac{1}{2}} = 67 \) d to 9.1 yr in water, based on measured rates for the reaction with hydroxyl radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991)

photooxidation \( t_{\frac{1}{2}} = 8.1–81 \) h in air, based on measured rate constant for the reaction of 1,3,5-trioxane with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

photooxidation \( t_{\frac{1}{2}} = 6.69–9.6 \) h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radicals (Howard 1990)

\[
k_{OH} = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1989)}
\]

\[
k_{OH(calc)} = 38.6 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, k_{OH(exptl)} = 10.9 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (SAR structure-activity relationship, Kwok & Atkinson 1995)}
\]

\[
k_{OH}^* = 9.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by relative rate method; } k_{OH} = 12.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be } 25 \text{ h at } 298 \pm 2 \text{ K; measured range 263–372 K (Moriarty et al. 2003)}
\]

Hydrolysis:

Biodegradation: aqueous aerobic \( t_{\frac{1}{2}} = 672–4320 \) h, based on unacclimated aerobic aqueous screening test data with confirmed resistance to biodegradation (Sasaki 1978; Kawasaki 1980; quoted, Howard et al. 1991); aqueous anaerobic \( t_{\frac{1}{2}} = 2688–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

\( t_{\frac{1}{2}}(\text{aerobic}) = 28 \text{ d; } t_{\frac{1}{2}}(\text{anaerobic}) = 110 \text{ d in natural waters (Capel & Larson 1995)}
\]

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance \( t_{\frac{1}{2}} < 0.24 \) h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
$t_{\frac{1}{2}} = 8.1–81$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991); $t_{\frac{1}{2}} = 6.69–9.6$ h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radical (Howard 1990).

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

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

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

Biota:

### Table 10.1.13.1
Reported vapor pressures of 1,4-dioxane at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Method</th>
<th>Hovorka et al. 1936</th>
<th>Crenshaw et al. 1938</th>
<th>Stull 1947</th>
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<tbody>
<tr>
<td></td>
<td>static method</td>
<td>ebulliometry-Hg manometer</td>
<td>summary of literature data</td>
<td>static method-Bourdon gauge</td>
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<tr>
<td>$t/°C$</td>
<td>P/Pa</td>
<td>$t/°C$</td>
<td>P/Pa</td>
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<td>2266</td>
<td>20</td>
<td>3853</td>
<td>–35.8</td>
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<tr>
<td>20</td>
<td>3746</td>
<td>25</td>
<td>4986</td>
<td>–12.8</td>
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FIGURE 10.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for dioxane.
10.1.2 HALOGENATED ETHERS

10.1.2.1 Epichlorohydrin

Common Name: Epichlorohydrin
Synonym: 1-chloro-2,3-epoxypropane, (chloromethyl)oxirane, α-epichlorohydrin, γ-chloropropylene oxide
Chemical Name: epichlorohydrin, 1-chloro-2,3-epoxypropane, α-epichlorohydrin, γ-chloropropylene oxide
CAS Registry No: 106-89-8
Molecular Formula: C₃H₅OCl
Molecular Weight: 92.524
Melting Point (°C):
-57.2 (Riddick et al. 1986; Howard 1989)
-26 (Lide 2003)
Boiling Point (°C):
118 (Lide 2003)
Density (g/cm³ at 20°C):
1.1807, 1.1746 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
78.4 (20°C, calculated-density)
90.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHᵥfus (kJ/mol):
Entropy of Fusion, ΔSᵥfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
65800 (20°C, selected, Riddick et al. 1986)
65800 (20°C, Krijgsheld & Van der Gen 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2400 (selected, Riddick et al. 1986)
log (P/kPa) = 6.5958 – 1587.9/(230 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
2192 (Daubert & Danner 1985)
log (P/kPa) = 6.5958 – 1587.9/(-43.15 + T/K); temp range 328–388 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 24.764 – 2.8846 × 10³/(T/K) – 5.6252 · log (T/K) – 1.1011 × 10⁻¹⁰ · (T/K)²; temp range 216–610 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
3.375 (calculated-P/C using Riddick et al. 1986 data)
Octanol/Water Partition Coefficient, log Kₐw:
0.30 (Krijgsheld & Van der Gen 1986)
0.45 (shake flask-GC, Deneer et al. 1988)
0.45 (recommended, Sangster 1993)
0.45 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
0.66 (estimated, Santodonato et al. 1980; quoted, Howard 1989)
Sorption Partition Coefficient, log Kₐc:
2.09 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2} \sim 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman 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: photooxidation $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989)

$$k_{OH}(calc) = 9.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{OH}(obs.) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)}$$

$$k_{OH} \geq 5.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with reference to n-butane for the gas phase reaction with OH radical at 23.3 \pm 0.9°C with an atmospheric lifetime of < 21 d for an average OH radical concentration of 1 \times 10^6 \text{ molecules/cm}^3 \text{ (Edney et al. 1986)}$$

$$k_{OH}(exptl) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{OH}(calc) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR, Atkinson 1987)}$$

$$k_{O3}(aq.) \leq 0.003 \text{ M}^{-1} \text{ s}^{-1} \text{ for direct reaction with ozone in water at pH 4.1 and 22°C, with } t_{1/2} - 130 \text{ d at pH 7 (Yao & Haag 1991).}$$


Biodegradation: aqueous aerobic $t_{1/2} = 168$–672 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Bridie et al. 1979; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$–2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photodecomposition $t_{1/2} = 16.0$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989); $t_{1/2} = 146$–1458 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991); atmospheric lifetime $< 21$ d due to reactions with OH radical (Edney et al. 1986).

Surface water: evaporation $t_{1/2} = 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989); $t_{1/2} = 168$–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); measured rate constant $k \leq 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.1 and 22°C, with $t_{1/2} - 130 \text{ d at pH 7 (Yao & Haag 1991).}$

Ground water: 336–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:
10.1.2.2 Chloromethyl methyl ether

\[ \text{Cl} \quad \text{O} \]

Common Name: Chloromethyl methyl ether
Synonym: chloromethyl ether, chloromethoxy methane, CMME, monochlorodimethyl ether
Chemical Name: chloromethyl methyl ether
CAS Registry No: 107-30-2
Molecular Formula: C₂H₅ClO, ClCH₂-O-CH₃
Molecular Weight: 80.513

Melting Point (°C):
–103.5 (Verschueren 1983; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
59.5 (Lide 2003)
Density (g/cm³ at 20°C):
1.0703 (Dean 1985)
1.0605 (Budavari 1989)
Molar Volume (cm³/mol):
75.2 (20°C, calculated-density)
81.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
decomposes (Verschueren 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
24900 (calculated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/P_kPa) = 6.259 - \frac{1240}{(-43.15 + T/K)}; \text{ temp range 290–332 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log \( K_{\text{oc}} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
Volatilization:
Photolysis:
Oxidation: photooxidation \( t_{1/2} = 22.7–227 \) h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: \( k = 21 \) h⁻¹ at pH 7 and 25°C with a calculated \( t_{1/2} = 2.0 \) min (Van Duuren et al. 1972; quoted, Ellington 1989);
\( t_{1/2} = 0.0108–0.033 \) h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991);
hydrolyzed very fast in aqueous solutions with \( t_{1/2} < 1.0 \) s (Verschueren 1983).
Biodegradation: aqueous aerobic \( t_{1/2} = 168–672 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
aqueous anaerobic \( t_{1/2} = 672–2688 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 22.7–227$ h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.0108–0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Ground water: $t_{1/2} = 0.0108–0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 0.0108–0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biota:
10.1.2.3 Bis(chloromethyl)ether

Common Name: Bis(chloromethyl)ether
Synonym: BCME, Bis-CME, chloro(chloromethoxy)methane, dichloromethylether, (dichloro-dimethyl)ether, sym-dichloromethyl ether, oxybis(chloromethane)
Chemical Name: chloromethyl ether, sym-dichloromethyl ether
CAS Registry No: 542-88-1
Molecular Formula: C₂H₄Cl₂O, ClCH₂-O-CH₂Cl
Molecular Weight: 114.958
Melting Point (°C):
Boiling Point (°C):
  106  (Lide 2003)
Density (g/cm³ at 20°C):
  1.328  (15°C, Weast 1982–83)
  1.315  (Verschueren 1983)
Molar Volume (cm³/mol):
  102.7  (calculated-Le Bas method at normal boiling point)
  87.4  (calculated-density, Stephenson & Malanowski 1987)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  22000  (calculated as per Moriguchi 1975 using Quayle 1953 data, Callahan et al. 1979)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  3999  (22°C, Dreisbach 1952)
  \[ \log (P/\text{mmHg}) = -3.4945 - 2.2305 \times 10^3/(T/K) + 6.774\log (T/K) - 1.7332 \times 10^{-2}(T/K) + 9.5511 \times 10^{-6}(T/K)^2; \]
  temp range 232–579 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
  21.27  (calculated-P/C, Mabey et al. 1982)
  213.18  (quoted from WERL Treatability Data, Ryan et al. 1988)
Octanol/Water Partition Coefficient, log K_{ow}:
  –0.38  (calculated, Radding et al. 1977)
  2.40  (calculated, Mabey et al. 1982)
Bioconcentration Factor, log BCF:
  1.041  (bluegill sunfish, Veith et al. 1980)
Sorption Partition Coefficient, log K_{OC}:
  1.20  (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:
  Volatilization:
  Photoysis:
  Oxidation: \( k << 360 \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and \( k = 3.0 \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical (Mabey et al. 1982)
  photooxidation \( t_{1/2} = 0.196–1.96 \text{ h} \), based on estimated rate constant for reaction with hydroxyl radical in air
Hydrolysis: hydrolyzed very fast in aqueous solution with half-life in the order of 10 s when extrapolated to pure water (Hammond & Alexander 1972; quoted, Verschueren 1983); rate constant \( k = 0.018 \text{ s}^{-1} \) with \( t_{1/2} = 38 \text{ s} \) (Tou et al. 1974; quoted, Callahan et al. 1979; Howard et al. 1991); hydrolysis \( t_{1/2} = 10–38 \text{ s} \) and will rapidly disappear from any aquatic system (Fishbein 1979; quoted, Howard 1989);

\[ k = 65 \text{ h}^{-1} \] at pH 7.0 at 20°C (quoted, Mabey et al. 1982).

Biodegradation: aqueous aerobic \( t_{1/2} = 168–672 \text{ h} \), based on scientific judgement; aqueous anaerobic \( t_{1/2} = 672–2688 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: \( t_{1/2} = 0.196–1.96 \text{ h} \), based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: \( t_{1/2} = 0.0106–0.106 \text{ h} \), based on estimated hydrolysis half-life in water (Howard et al. 1991).

Ground water: \( t_{1/2} = 0.0106–0.106 \text{ h} \), based on estimated hydrolysis in water (Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} < 10 \text{ d} \), via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

\( t_{1/2} = 0.0106–0.106 \text{ h} \), based on estimated hydrolysis half-life in water (Howard et al. 1991).

Biota:
10.1.2.4 Bis(2-chloroethyl)ether

Common Name: Bis(2-chloroethyl)ether
Synonym: 2-chloroethyl ether, 1,1’-oxybis(2-chloroethane), bis(β-chloroethyl)ether, Chlorex, 1-chloro-2-(β-chloroethoxy)-ethane, β,β’-dichloroethyl ether, 2,2’-dichloroethyl ether, di(2-chloroethyl)ether, di(chloroethyl)ether, dichlorodiethyl ether, sym-dichlorodiethyl ether
Chemical Name: 2-chloroethyl ether, bis(β-chloroethyl)ether, 1-chloro-2-(β-chloroethoxy)-ethane
CAS Registry No: 111-44-4
Molecular Formula: C₄H₈Cl₂O, ClCH₂CH₂-O-CH₂CH₂Cl
Molecular Weight: 143.012

Melting Point (°C):
-51.9 (Lide 2003)

Boiling Point (°C):
178.5 (Lide 2003)

Density (g/cm³ at 20°C):
1.2200 (Verschueren 1983)
1.2192 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm³/mol):
117.3 (20°C, calculated-density)
147.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_fus (kJ/mol):
8.66 (Riddick et al. 1986)

Entropy of Fusion, ΔS_fus (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
10200 (20°C, Du Pont 1966; Verschueren 1983)
17195 (shake flask-LSC, Veith et al. 1980)
10200 (20°C, Riddick et al. 1986)
10400*, 10300 (20°C, 31°C, shake flask-GC/TC, measured range 0–91.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
156.2 (Antoine eq. regression, temp range 23.5–178.5°C, Stull 1947)
94.64, 186 (20, 25°C, Verschueren 1977,1983)
207 (selected, Riddick et al. 1986)
log (P/kPa) = 7.2289 – 2359.6/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
143.6 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
857.1 (calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
28.97 (calculated-P/C, Lyman et al. 1982; Howard 1989)
1.320 (20°C, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{ow}:
1.58 (calculated, Leo et al. 1971)
1.12 (shake flask-LSC, Veith et al. 1980)
1.29 (shake flask, Hansch & Leo 1985)
1.29 (recommended, Sangster 1993)
1.29 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
- 1.041 (bluegill sunfish, Barrows et al. 1980)
- 1.040 (bluegill sunfish, LSC-14C, Veith et al. 1980; Veith & Kosian 1983)
- 0.964 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
- 1.15 (calculated, Sabljic 1987)

Sorption Partition Coefficient, log K_{OC}:
- 1.38 (soil, calculated-S, Lyman et al. 1982)
- 1.14 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

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

   Volatilization: calculated t_{1/2} = 5.78 d (as per Mackay & Wolkoff 1973 by Durkin et al. 1975);
   t_{1/2} = 3.5, 4.4 and 180.5 d for the streams, rivers and lakes, respectively, were estimated using Henry’s law constant (Lyman et al. 1982; quoted, Howard 1989).

   Photolysis:
   Oxidation: photooxidation t_{1/2} = 4.0 h, based on an estimated half-life for ethyl ether in the smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979); k << 360 M^{-1}h^{-1} for the reaction with singlet oxygen and k = 24.0 M^{-1}h^{-1} for the reaction with peroxy radical (Mabey et al. 1982);
   photooxidation t_{1/2} = 9.65–96.5 h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

   Hydrolysis: t_{1/2} = 40.0 d was estimated at pH 7 from ethyl chloride data in water at an unspecified temperature (Brown et al. 1975; quoted, Howard 1989); t_{1/2} = 0.5–2.0 yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);
   first-order hydrolysis t_{1/2} = 22 yr, based on neutral hydrolysis rate constant at 20°C which was extrapolated from data for hydrolysis of dioxane at 100°C (Mabey et al. 1982; quoted, Howard et al. 1991); k = 2.6 \times 10^{-4} h^{-1} at pH 7 and 25°C with a calculated t_{1/2} = 3.0 yr (Ellington et al. 1987; quoted, Ellington 1989).

   Biodegradation: aqueous aerobic t_{1/2} = 672–4320 h, based on river die-away test data (Ludzack & Ettinger 1963 and Doljido 1979; 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: k = 3 \times 10^{-9} mL cell^{-1} h^{-1} for the bacterial transformation in water (Mabey et al. 1982).

   Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:

Half-Lives in the Environment:

   Air: atmospheric t_{1/2} = 13.44 h was estimated for the reaction with OH radical (GEMS 1986; quoted, Howard 1989);
   photooxidation t_{1/2} = 9.65–96.5 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} = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

   Biota: t_{1/2} > 4.0 d but less than 7.0 d in fish tissues (Barrows et al. 1980).
TABLE 10.1.2.4.1
Reported aqueous solubilities of bis(2-chloroethyl) ether at various temperatures

Stephenson 1992

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FIGURE 10.1.2.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bis(2-chloroethyl)ether.
10.1.2.5 Bis(2-chloroisopropyl)ether

Common Name: Bis(2-chloroisopropyl)ether
Synonym: bis(2-chloro-1-methylethyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether, 2,2′-dichloroisopropyl ether, 2,2′-oxybis(1-chloropropane)
Chemical Name: bis(2-chloroisopropyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether
CAS Registry No: 108-60-1
Molecular Formula: C₆H₁₂Cl₂O, ClCH₂CH(CH₃)-O-CH(CH₃)CH₂Cl
Molecular Weight: 171.064
Melting Point (°C): –97 (Weast 1977; Verschueren 1983)
Boiling Point (°C):
187  (Lide 2003)
Density (g/cm³ at 20°C):
1.1100  (Verschueren 1983)
1.1122  (Dean 1985)
Molar Volume (cm³/mol):
154.1  (20°C, calculated-density)
193.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1700*  (room. temp., Verschueren 1977,1983)
2450*, 2370 (19.1°C, 31.0°C, shake flask-GC, measured range 9.5–91.4°C, Stephenson 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
103.95  (Antoine eq. regression, temp range 24.7–180°C, Stull 1947)
113.31  (20°C, Verschueren 1977,1983)
112.30  (28.85°C, Antoine eq., Stephenson & Malanowski 1987)
log (P_v/Pa) = 6.68233 – 1856.14/(-58.793 + T/K); temp range 302–456 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
11.14  (20°C, calculated-P/C, Mabey et al. 1982)
11.40  (calculated-P/C from Verschueren 1977/83 data)
116.5  (quoted from WERL Treatability Data, Ryan et al. 1988)
Octanol/Water Partition Coefficient, log KOW:
2.58  (calculated, Leo et al. 1971)
2.10  (calculated, Mabey et al. 1982)
2.48  (HPLC-RT correlation, Kawamoto & Urano 1989)
2.48  (recommended, Sangster 1993)
Bioconcentration Factor, log BCF:
1.544  (microorganisms-water, calculated-KOW, Mabey et al. 1982)
Sorption Partition Coefficient, log KOC:
1.785  (sediment-water, calculated-KOW, Mabey et al. 1982)
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

Volatilization: calculated \( t_{1/2} = 1.37 \) d (calculated as per Mackay & Wolkoff 1973, Durkin et al. 1975; quoted, Callahan et al. 1979).

Photolysis:

Oxidation: photooxidation \( t_{1/2} = 4.0 \) h, based on estimated half-life for ethyl ether in a smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

\( k \ll 360 \) M\(^{-1}\) h\(^{-1}\) for the reaction with singlet oxygen and \( k = 2.0 \) M\(^{-1}\) h\(^{-1}\) for the reaction with peroxy radical (Mabey et al. 1982).

Hydrolysis: \( t_{1/2} = 0.5–2.0 \) yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

\( k = 4 \times 10^{-6} \) h\(^{-1}\) at pH 7.0 and 25°C (Mabey et al. 1982).

Biodegradation: aqueous aerobic \( t_{1/2} = 432–4320 \) h, based on river die-away test data (Kleopfer & Fairless 1972; quoted, Howard et al. 1991) and aerobic soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991); aqueous anaerobic \( t_{1/2} = 1728–17280 \) h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

Half-Lives in the Environment:

Air: \( t_{1/2} = 4.61–46.1 \) h, based on photooxidation half-life in air (Howard et al. 1991).

Surface water: estimated \( t_{1/2} = 3.1 \) d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

\( t_{1/2} = 432–4320 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: \( t_{1/2} = 864–8640 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} = 432–4320 \) h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 10.1.2.5.1</th>
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<tr>
<td>Report aqueous solubilities of bis(2-chloroisopropyl) ether at various temperatures</td>
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FIGURE 10.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bis(2-chloroisopropyl)ether.

$\ln x$ vs. $1/T$
### 2-Chloroethyl vinyl ether

Common Name: 2-Chloroethyl vinyl ether  
Synonym: (2-chloroethoxy)-ethene, β-chloroethyl vinyl ether, vinyl 2-chloroethyl ether  
Chemical Name: β-chloroethyl vinyl ether, 2-chloroethyl vinyl ether, vinyl 2-chloroethyl ether  
CAS Registry No: 110-75-8  
Molecular Formula: C₄H₇Cl₂O, ClCH₂CH₂-O-CH=CH₂  
Molecular Weight: 106.551  
Melting Point (°C):  
-70 (Lide 2003)  
Boiling Point (°C):  
Density (g/cm³ at 20°C):  
1.0475 (Weast 1982–83)  
1.0480 (Dean 1985)  
Molar Volume (cm³/mol):  
101.7 (20°C, calculated-density)  
119.6 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ∆H_fus (kJ/mol):  
Entropy of Fusion, ∆S_fus (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
15000 (calculated as per Moriguchi 1975, Callahan et al.)  
6000 (Dean 1985)  
Vapor Pressure (Pa at 25°C or as indicated):  
3566 (20°C, calculated, Dreisbach 1952)  
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):  
0.0253 (20–25°C, calculated-P/C, Mabey et al. 1982)  
24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)  
Octanol/Water Partition Coefficient, log K_{OW}:  
1.28 (calculated as per Leo et al. 1971, Callahan et al. 1979)  
1.14 (calculated, Mabey et al. 1982)  
Bioconcentration Factor, log BCF:  
0.672 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)  
Sorption Partition Coefficient, log K_{OC}:  
0.820 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)  
Environmental Fate Rate Constants, k, and Half-Lives, t_½:  
Volatilization:  
Photolysis:  
Oxidation: photooxidation t_½ = 30 min, based on half-life estimated for 2-methyl-2-butene from smog chamber data (Altschuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);  
k = 1 × 10^{10} M^{-1}·h^{-1} for singlet oxygen and k = 34 M^{-1}·h^{-1} for peroxy radical (Mabey et al. 1982).  
Hydrolysis: k = 4.4 × 10^{-10} s^{-1}, minimum rate at pH 7 and 25°C in pure water with a maximum t_½ = 0.48 yr (Jones & Wood 1964; quoted, Callahan et al. 1979);  
k ~ 4 × 10^{-6} h^{-1} at pH 7.0 and 25°C with reference to that of bis(2-chloroethyl)ether (Mabey et al. 1982).
Biodegradation:
Biotransformation: $k = 1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacterial transformation to water (Mabey et al. 1982).

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

Half-Lives in the Environment:
Soil: $t_{1/2} < 10$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).
10.1.2.7 Bis(2-chloroethoxy)methane

\[
\text{Cl} = O - O = \text{Cl}
\]

Common Name: Bis(2-chloroethoxy)methane
Synonym: bis(\(\beta\)-chloroethyl)formal, \(\beta, \beta\)-dichlorodiethyl formal, dichlorodiethyl methylal
Chemical Name: bis(2-chloroethoxy)methane
CAS Registry No: 111-91-1
Molecular Formula: C\(_5\)H\(_{10}\)Cl\(_2\)O\(_2\), ClCH\(_2\)CH\(_2\)-O-CH\(_2\)-O-CH\(_2\)CH\(_2\)Cl
Molecular Weight: 173.037
Melting Point (°C):
Boiling Point (°C): 215 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
Molar Volume (cm\(^3\)/mol):
180.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C):
81000 (calculated as per Moriguchi 1975, Callahan et al. 1979;)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
< 13.3 (calculated as per Dreisbach 1952 using data of Webb et al. 1962, Callahan et al. 1979)
21.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P\(_r\)/Pa) = 7.54778 – 2641.33/(–11.518 + T/K); temp range 326–486 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C or as indicated):
0.0284 (20–25°C, calculated-P/C, Mabey et al. 1982)
0.0273 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
1.260 (calculated as per Leo et al. 1971, Callahan et al. 1979; Ryan et al. 1988)
1.029 (calculated, Mabey et al. 1982)

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

Sorption Partition Coefficient, log \(K_{\text{OC}}\):
0.716 (sediment-water, calculated-\(K_{\text{OW}}\), Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, \(t_{1/2}\):
Volatilization:
Photolysis:
Oxidation: \(k < << 360\) M\(^{-1}\) h\(^{-1}\) for singlet oxygen and \(k = 52\) M\(^{-1}\) h\(^{-1}\) for peroxy radical (Mabey et al. 1982).
Hydrolysis: minimum rate \(k = 2.53 \times 10^{-6}\) L mol\(^{-1}\) s\(^{-1}\) for acid-catalyzed hydrolysis of the acetal linkage at 25°C (Kankaanperä 1969; quoted, Callahan et al. 1979; Mabey et al. 1982);
\(t_{1/2} = 0.5–2.0\) yr, based on data of Dilling et al. 1975 on chlorinated ethanes and propanes (quoted, Callahan et al. 1979);
estimated rate constant \(k \sim 4 \times 10^{-6}\) h\(^{-1}\) at pH 7.0 and 25°C by analogy to bis(2-chloroethyl)ether (Mabey et al. 1982).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Soil: $t_{1/2} > 50$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).
10.1.3 AROMATIC ETHERS

10.1.3.1 Anisole (Methoxybenzene)

Common Name: Anisole
Synonym: methoxybenzene
Chemical Name: anisole, methoxybenzene, methyl phenyl ether
CAS Registry No: 100-66-3
Molecular Formula: C₇H₈O, C₆H₅OCH₃
Molecular Weight: 108.138
Melting Point (°C): –37.13 (Lide 2003)
Boiling Point (°C): 153.7 (Lide 2003)
Density (g/cm³ at 20°C):
- 0.99402, 0.98932 (20°C, 25°C, Dreisbach & Martin 1949)
- 0.9940, 0.9893 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
- 108.8 (20°C, calculated-density)
- 127.3 (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, 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):
- 1514 (shake flask-UV, McGowan et al. 1966)
- 1536 (shake flask-UV, Vesala 1974)
- 2030*, 1860 (20°C, 29.7°C, shake flask-GC/TC, measured range 0–90.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 497* (calculated-Antoine eq. regression, temp range 5.4–155.5°C, Stull 1947)
  log (P/mmHg) = 7.35950 – 1718.7/(230 + t°C) (Antoine eq., temp range 73–154°C, Dreisbach & Martin 1949)
- 6287* (73.34°C, ebulliometry, measured range 73.34–153.75°C, Dreisbach & Shrader 1949)
  log (P/mmHg) = 7.05236 – 1489.756/(203.543 + t°C); temp range 109.876–164.114°C (Antoine eq., ebullimetric measurements, Collerson et al. 1965)
- log (P/mmHg) = 22.84299 – 3033.20/(T/K) – 4.88720·log (T/K); temp range 346.49–415.52 K (Cox eq., Chao et al. 1983)

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log (P/mmHg) = 7.05269 – 1489.99/(203.57 + t/°C); temp range 110–164°C (Antoine eq., Dean 1985, 1992)

472 (selected, Riddick et al. 1986)

log (P/kPa) = 6.17595 – 1489.502/(203.573 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (PL/kPa) = 6.17622 – 1489.957/(-69.525 + T/K); temp range 382–437 K (Antoine eq., Stephenson & Malanowski 1987)

204, 383 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

log (P/mbar) = 7.11773 – 1451.742/[(T/K) –73.252]; temp range 382–429 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)

log (P/mmHg) = –8.1053 – 2.5386 × 10^3/(T/K) + 9.0289·log (T/K) – 2.0426 × 10^–2·(T/K) + 1.0536 × 10^–5·(T/K)^2; temp range 236–642 K (vapor pressure eq., Yaws 1994)

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

430.8 (exptl. 1/K AW = C W/CA, Hine & Mookerjee 1975)

430.8, 358.3 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

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

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

2.04 (shake flask-UV, Rogers & Cammarata 1969)

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

2.08 (Hansch & Leo 1979)

2.24 (HPLC-k′ correlation, Haky & Young 1984)

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

2.15 (HPLC-RT correlation, Minick et al. 1988)

2.01 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

2.11 (recommended, Sangster 1989, 1993)

2.17 (dual-mode centrifugal partition chromatography, Gluck 1990)

1.67, 1.79 (shake flask-UV/VIS spec.: 25, 60°C, Kramer & Henze 1990)

2.11 (recommended, Hansch et al. 1995)

2.41, 2.31, 2.58, 2.55 (HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsakya et al. 1995)

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

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

Bioconcentration Factor, log BCF:

1.34 (Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC}:

6.50 (soil, calculated-MCI 1χ, Sabljic et al. 1995)

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

Volatilization:

Photolysis: rate constant k = 1.054 × 10^{-2} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)

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_0 with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = (1.57 ± 0.24) × 10^{-11} cm^3 molecule^{-1} s^{-1} at 299 K, measured range 299–435 K (overall rate constant, flash photolysis-resonance fluorescence technique, Perry et al. 1977)

k_{OH} = 1.57 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1985; quoted, Sabljic & Güsten 1990)

k_{NO_3} = 9.0 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (re-evaluated value, Atkinson et al. 1987)

k_{OH} = 1.35 × 10^{-12} cm^3 molecule^{-1} s^{-1} in air, extrapolated from lit. data to 25°C (Dilling et al. 1988)

k_{NO_3} = 2.08 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

k_{OH} = (14.1 – 19.6) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. to 299.9 K (Atkinson 1989)

Hydrolysis:

Biodegradation:
Biotransformation: degradation \( k = 2.86 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1} \) in pure culture system (Banerjee et al. 1984).

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

Half-Lives in the Environment:
Air: disappearance \( t_\text{1/2} < 0.24 \text{ h} \) from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

### TABLE 10.1.3.1.1
Reported aqueous solubilities of anisole at various temperatures

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**FIGURE 10.1.3.1.1** Logarithm of mole fraction solubility \((\ln x)\) versus reciprocal temperature for anisole.

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**TABLE 10.1.3.1.2**

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

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

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<th>t/°C</th>
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**Summary of literature data**

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**Dreisbach & Martin 1949**

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**Ambrose et al. 1976**

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**Dreisbach & Shrader 1949**

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**Collerson et al. 1965**

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**Antoine eq.**

- **A**: 7.3595
- **B**: 1718.7
- **C**: 230
- **bp/°C**: 153.75
- **mp/°C**: -37.38

- **Antoine eq.**
  - **A**: 6.17595
  - **B**: 705236
  - **C**: 1489.502
  - **bp/°C**: 150.429
  - **mp/°C**: -37.38

- **Kirchhoff eq.**
  - **eq. 4**: P/mmHg
    - **A**: 22.842 99
    - **B**: 3033.2
    - **C**: 4.8872
  - **∆H_v/(kJ mol⁻¹)** = 39.04
FIGURE 10.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for anisole.
10.1.3.2 2-Chloroanisole

![Chemical Structure](image)

Common Name: 2-Chloroanisole  
Synonym: 1-chloro-2-methoxybenzene  
Chemical Name: 2-chloroanisole  
CAS Registry No: 766-51-8  
Molecular Formula: C₇H₇ClO, C₆H₄Cl(OCH₃)  
Molecular Weight: 142.583  
Melting Point (°C): liquid  
-26.8 (Stephenson & Malanowski 1987; Lide 2003)  
Boiling Point (°C):  
198.5 (Lide 2003)  
Density (g/cm³ at 20°C):  
1.1911 (Lide 2003)  
Molar Volume (cm³/mol):  
119.7 (20°C, calculated-density)  
148.2 (Le Bas method-calculated at normal boiling point)  
Enthalpy of Vaporization, ∆HV (kJ/mol):  
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):  
Enthalpy of Fusion, ∆Hfus (kJ/mol):  
Entropy of Fusion, ∆Sfus (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
490 (shake flask-HPLC/UV, Lun et al. 1995)  
766 (liquid S_L, RP-HPLC-k’ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)  
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):  
6287 (115.13°C, ebulliometry, measured range 115.13–186.19°C, Dreisbach & Shrader 1949)  
log (P/mmHg) = 7.54073 – 2012.4/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)  
log (P/kPa) = 6.25236 – 1660.008/(189.207 + t°C), temp range 115.13–186.19°C (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublík et al. 1984)  
0.0594 (P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P_L/kPa) = 6.66563 – 2012.4/(–43.15 + T/K), temp range 388–460 K, (Antoine eq., Stephenson & Malanowski 1987)  
0.0302 (liquid P_L, GC-RT correlation, Pfeifer et al. 2001)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
9.50 (calculated-P_L/C_L, Pfeifer et al. 2001)  
Octanol/Water Partition Coefficient, log Kow:  
2.68 (shake flask-UV, Nakagawa et al. 1992)  
2.50 (shake flask-HPLC/UV both phases, Lun et al. 1995)  
2.72 (RP-HPLC-k’ correlation, Pfeifer et al. 2001)  
Octanol/Air Partition Coefficient, log Koa:  
3.13 (calculated-K_ow/K_aw, Pfeifer et al. 2001)  
Bioconcentration Factor, log BCF or log Kg:  
Sorption Partition Coefficient, log Koc:
10.1.3.3 3-Chloroanisole

Common Name: 3-Chloroanisole
Synonym:
Chemical Name:
CAS Registry No: 2845-89-8
Molecular Formula: C₇H₇ClO, C₆H₄Cl(OCH₃)
Molecular Weight: 142.583
Melting Point (°C): liquid
Boiling Point (°C):
  193.5  (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
  148.2  (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₘₖₗ (kJ/mol):
Enthalpy of Fusion, ΔHₚ (kJ/mol):
Entropy of Fusion, ΔSₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  235  (shake flask-HPLC/UV, Lun et al. 1995)
  231  (liquid Sₗ, RP-HPLC-k’ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
  0.0282  (liquid Pₗ, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
  21.4  (calculated-Pₗ/Cₗ, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log Kₗₜₜ:
  2.60  (shake flask-HPLC/UV both phases, Lun et al. 1995)
  3.09  (RP-HPLC-k’ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log Kₗₜₚ:
  3.15  (calculated-Kₗₜₚ/K₄ₜₚ, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log Kₚ:
Sorption Partition Coefficient, log Kₜₚ:
10.1.3.4 4-Chloroanisole

Common Name: 4-Chloroanisole
Synonym: 1-chloro-4-methoxy-benzene
Chemical Name: 4-chloroanisole
CAS Registry No: 623-12-1
Molecular Formula: C₇H₇ClO, C₆H₄Cl(OCH₃)
Molecular Weight: 142.583
Melting Point (°C):
   < −18 (Lide 2003)
Boiling Point (°C):
   197.5 (Lide 2003)
Density (g/cm³ at 20°C):
   1.201 (Lide 2003)
Molar Volume (cm³/mol):
   118.7 (20°C, calculated-density)
   148.2 (Le Bas method-calculated at normal boiling point)
Enthalpy of Fusion, ΔH₅₆ (kJ/mol):
Entropy of Fusion, ΔS₅₆ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₅₆ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   237 (shake flask-HPLC/UV, Lun et al. 1995)
   312 (liquid Sₗ, RP-HPLC-k’ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
   0.0324 (liquid Pₗ, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
   18.2 (calculated-Pₗ/Cₗ, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log Kₐw:
   2.78 (23°C, shake flask-LSC, Banerjee et al. 1980)
   2.78 (recommended, Sangster 1993)
   2.70 (shake flask-HPLC/UV both phases, Lun et al. 1995)
   3.00 (RP-HPLC-k’ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log Kₐa:
   3.13 (calculated-Kₐw/Kₐw, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log Kₜ:
Sorption Partition Coefficient, log Kₜc:
Environmental Fate Rate Constants, k, and Half-Lives, tₜ:
   Biodegradation: degradation rate constants k = 2.29 × 10⁻¹⁸ mol cell⁻¹ h⁻¹ from pure culture studies (Banerjee et al. 1984).
   Half-Lives in the Environment:
10.1.3.5 2,3-Dichloroanisole

Common Name: 2,3-Dichloroanisole
Synonym: 
Chemical Name: 
CAS Registry No: 1984-59-4
Molecular Formula: C₇H₆Cl₂O, C₆H₃Cl₂(OCH₃)
Molecular Weight: 177.028
Melting Point (°C): 
Boiling Point (°C): 32 (Lun et al. 1995; Lide 2003)
Density (g/cm³): 
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₛₛₙₐₙ (kJ/mol):
Enthalpy of Fusion, ΔHₕₙₜ (kJ/mol):
Entropy of Fusion, ΔSₕₙₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕₙₜ = 56 J/mol K), F: 0.854 (mp at 32°C)
Water Solubility (g/m³ or mg/L at 25°C): 
Vapor Pressure (Pa at 25°C): 
Henry’s Law Constant (Pa m³/mol at 25°C): 
Octanol/Water Partition Coefficient, log Kₒₕₔₜ:
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₒₜₑ:
Environmental Fate Rate Constants, k, and Half-Lives, tₜₑ, or Lifetimes, τ:
Half-Lives in the Environment:
10.1.3.6 2,6-Dichloroanisole

Common Name: 2,6-Dichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 1984-65-2
Molecular Formula: C₇H₆Cl₂O, C₆H₃Cl₂(OCH₃)
Molecular Weight: 177.028
Melting Point (°C):
  10 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  169.1 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₛₒₜₜ (kJ/mol):
Enthalpy of Fusion, ΔHₕₜₜ (kJ/mol):
Entropy of Fusion, ΔSₕₜₜ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  13.12 (shake flask-GC/ECD, Lun et al. 1995)
  21.8 (liquid Sₗ, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
  0.0110 (liquid Pₗ, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
  113.7 (calculated-Pₗ/Cₗ, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log Kₐₒₜₜ:
  2.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  3.14 (shake flask-HPLC/UV both phases, Lun et al. 1995)
  3.10 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log Kₐₒₜₜ:
  2.53 (calculated-Kₒₒₜₜ/Kₒₐₜₜ, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log Kₐₕ:
Sorption Partition Coefficient, log Kₒₑ:
Environmental Fate Rate Constants, k, and Half-Lives, tₜₜ:
Half-Lives in the Environment:
10.1.3.7 2,3,4-Trichloroanisole

Common Name: 2,3,4-Trichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 54135-80-7
Molecular Formula: C₇H₅Cl₃O, C₆H₂Cl₃(OCH₃)
Molecular Weight: 211.473
Melting Point (°C): 70 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
    190.0 (Le Bas method-calculated 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: 0.362 (mp at 70°C)
Water Solubility (g/m³ or mg/L at 25°C):
    10.8 (shake flask-GC/ECD, Lun et al. 1995)
    22.1 (supercooled liquid S_L, RP-HPLC-k′ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
    0.263 (supercooled liquid P_L, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
    74.7 (calculated-P_L/C_L, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log K_{OW}:
    3.74 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
    4.03 (shake flask-GC/ECD, both phases, Lun et al. 1995)
    3.92 (RP-HPLC-k′ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log K_{OA}:
    3.44 (calculated-K_{OW}/K_{AW}, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log K_{B}:
    3.09 (guppy, concn ratio of C_fish/C_water, Opperhuizen & Voors 1987)
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, τ, or Lifetimes, τ:
    Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):
    k₁ = 1450 mL g⁻¹ d⁻¹; k₂ = 1.9 d⁻¹ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)
    Half-Lives in the Environment:
10.1.3.8 2,4,6-Trichloroanisole

Common Name: 2,4,6-Trichloroanisole
Synonym:
Chemical Name:
CAS Registry No: 87-40-1
Molecular Formula: C_{7}H_{5}Cl_{3}O, C_{6}H_{2}Cl_{3}(OCH_{3})
Molecular Weight: 211.473
Melting Point (°C): 61.5 (Lide 2003)
Boiling Point (°C): 241 (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
190.0 (Le Bas method-calculated 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: 0.438 (mp at 61.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
13.2 (shake flask-GC/ECD, Lun et al. 1995)
14.6 (supercooled liquid S₁, RP-HPLC-k’ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
2.065 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0724 (supercooled liquid P₁, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
218.7 (calculated-P₁/C₁, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log K_{ow}:
5.20 (HPLC-relative retention time correlation, Neilson et al. 1984)
4.11 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
3.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
4.02 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.05 (RP-HPLC-k’ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log K_{oa}:
3.10 (calculated-K_{ow}/K_{aw}, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log K_{b}:
3.90 (zebra fish, Neilson et al. 1984)
2.86 (guppy, concn ratio of C_{fish}/C_{water}, Opperhuizen & Voors 1987)
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{½}:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):
k₁ = 1600 mL g⁻¹ d⁻¹; k₂ = 2.5 d⁻¹ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)
Half-Lives in the Environment:
Biota: biological t_{½} < 1 d for all trichloro congeners (guppy, Opperhuizen & Voors 1987)
10.1.3.9 2,3,4,5-Tetrachloroanisole

Common Name: 2,3,4,5-Tetrachloroanisole
Synonym:
Chemical Name:
CAS Registry No: 938-86-3
Molecular Formula: C$_7$H$_4$Cl$_4$O, C$_6$HCl$_4$(OCH$_3$)
Molecular Weight: 245.918
Melting Point (°C): 88 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm$^3$):
Molar Volume (cm$^3$/mol):
210.9 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at 88°C)
Water Solubility (g/m$^3$ or mg/L at 25°C):
1.35 (shake flask-GC/ECD, Lun et al. 1995)
2.76 (supercooled liquid $S_L$, RP-HPLC-$k'$ correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
1.202 (supercooled liquid $P_L$, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m$^3$/mol at 25°C):
153.0 (calculated-$P_L/C_L$, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log $K_{ow}$:
4.51 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.50 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.57 (RP-HPLC-$k'$ correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log $K_{oa}$:
3.78 (calculated-$K_{ow}/K_{aw}$, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log $K_b$:
3.67 (guppy, concn ratio of $C_{fish}/C_{water}$, Opperhuizen & Voors 1987)
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$, or Lifetimes, $\tau$:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  $k_1 = 940$ mL g$^{-1}$ d$^{-1}$; $k_2 = 0.42$ d$^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)
Half-Lives in the Environment:
  - Biota: biological $t_{1/2} \sim 1$–4 d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)
10.1.3.10 2,3,5,6-Tetrachloroanisole

Common Name: 2,3,5,6-Tetrachloroanisole
Synonym:
Chemical Name:
CAS Registry No: 6936-40-9
Molecular Formula: C₇H₄Cl₄O, C₆HCl₄(OCH₃)
Molecular Weight: 245.918
Melting Point (°C):
84 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
210.9 (Le Bas method-calculated at normal boiling point)
Enthalpy of Fusion, ΔHₜₚ (kJ/mol):
Entropy of Fusion, ΔSₜₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₚ = 56 J/mol K), F: 0.264 (mp at 84°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.82 (shake flask-GC/ECD, Lun et al. 1995)
3.64 (supercooled liquid Sₐ, RP-HPLC-k' correlation, using chlorobenzene as reference compound standard, Pfeifer et al. 2001)
Vapor Pressure (Pa at 25°C):
0.427 (supercooled liquid Pₐ, GC-RT correlation, Pfeifer et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
318.4 (calculated-Pₐ/Cₐ, Pfeifer et al. 2001)
Octanol/Water Partition Coefficient, log Kₐₜₜ:
4.68 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
4.40 (shake flask-GC/ECD, both phases, Lun et al. 1995)
4.52 (RP-HPLC-k' correlation, Pfeifer et al. 2001)
Octanol/Air Partition Coefficient, log Kₐₚ:
3.41 (calculated-Kₐₚ/Kₐₚ, Pfeifer et al. 2001)
Bioconcentration Factor, log BCF or log Kᵦ:
3.69 (guppy, concn ratio of Cᵦ/Cₜₜ, Opperhuizen & Voors 1987)
Sorption Partition Coefficient, log Kₜₜ:
Environmental Fate Rate Constants, k, and Half-Lives, tₜₜ, or Lifetimes, τ:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):
k₁ = 1480 mL g⁻¹ d⁻¹; k₂ = 0.44 d⁻¹ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)
Half-Lives in the Environment:
Biota: biological tₐᵦ ~ 1–4 d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)
10.1.3.11 Veratrole (1,2-Dimethoxybenzene)

Common Name: Veratrole
Synonym: 1,2-dimethoxybenzene
Chemical Name: 1,2-dimethoxybenzene
CAS Registry No: 91-16-7
Molecular Formula: C₈H₁₀O₂, C₆H₄(OCH₃)₂
Molecular Weight: 138.164
Melting Point (°C):
22 (Stephenson & Malanowski 1987)
22.5 (Lide 2003)
Boiling Point (°C):
206.7 (Stephenson & Malanowski 1987)
206 (Lide 2003)
Density (g/cm³):
Molar Volume (cm³/mol):
127.1 (calculated-density)
158.6 (Le Bas method-calculated at normal boiling point)
Enthalpy of Fusion, ΔHₚₑₜ (kJ/mol):
Entropy of Fusion, ΔSₚₑₜ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
7160*, 7060 (19.9, 31°C, shake flask-GC, measured range 19.9–91.8°C, Stephenson 1992)
6690 (shake flask-HPLC/UV, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):
log (P/vkPa) = 8.705 – 3492/(T/K), temp range not specified (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₗₚₗ:
1.79 (Log P Database, Hansch & Leo 1987, quoted, Sangster 1993)
1.79 (HPLC-RT correlation, average value, Ritter et al. 1994)
1.60 (recommended, Hansch et al. 1995)
2.18 (shake flask-HPLC/UV both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, log Kₗₚₐ:
Bioconcentration Factor, log BCF or log Kₗₗ:
Sorption Partition Coefficient, log Kₗₜₗ:
Environmental Fate Rate Constants, k, and Half-Lives, tₛ:
TABLE 10.1.3.11.1
Reported aqueous solubilities of veratrole at various temperatures

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<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
</tr>
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<tr>
<td>19.9</td>
<td>7160</td>
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<td>31</td>
<td>7060</td>
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<td>41.1</td>
<td>7230</td>
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<td>9700</td>
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<tr>
<td>91.8</td>
<td>10730</td>
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</table>

FIGURE 10.1.3.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for veratrole.
10.1.3.12 4,5-Dichloroveratrole

Common Name: 4,5-dichloroveratrole
Synonym:
Chemical Name:
CAS Registry No: 2772-46-5
Molecular Formula: C₈H₈Cl₂O₂, C₆H₂Cl₂(OCH₃)₂
Molecular Weight: 207.054
Melting Point (°C):
83  (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
200.4  (Le-Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.27 (mp at 83°C)
Water Solubility (g/m³ or mg/L at 25°C):
71.9  (shake flask-HPLC/UV, Lun et al. 1995)
72.6  (shake flask-GC/ECD, Lun et al. 1995)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
3.11  (shake flask-GC/ECD, both phases, Lun et al. 1995)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kb:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
### 3,4,5-Trichloroveratrole

**Chemical Name:** 3,4,5-trichloroveratrole  
**Synonym:**  
**CAS Registry No:** 16766-29-3

**Molecular Formula:** C₈H₇Cl₃O₂, C₆HCl₃(OCH₃)₂  
**Molecular Weight:** 241.499

**Melting Point (°C):**  
66 (Lun et al. 1995)

**Boiling Point (°C):**

**Density (g/cm³):**

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

**Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):**

**Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):**

**Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):**

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

**Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \)), \( F \):** 0.396 (mp at 66°C)

**Water Solubility (g/m³ or mg/L at 25°C):**  
2.50 (shake flask-GC, Neilson et al. 1984)  
10.3 (shake flask-GC/ECD, Lun et al. 1995)

**Vapor Pressure (Pa at 25°C):**

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

**Octanol/Water Partition Coefficient, log \( K_{ow} \):**  
4.60, 5.25 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)  
4.01 (shake flask-GC/ECD, both phases, Lun et al. 1995)

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

**Bioconcentration Factor, log \( BCF \) or log \( K_b \):**  
3.50, 3.30 (zebra fish, calculated, Neilson et al. 1984)

**Sorption Partition Coefficient, log \( K_{OC} \):**  
3.20 (sediment, \( K_p = 1.6 \text{ ml/(kg of organic C)} \), batch sorption equilibrium, Remberger et al. 1986)

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

Half-Lives in the Environment:
10.1.3.14 Tetrachloroveratrole

Common Name: Tetrachloroveratrole
Synonym: 1,2,3,4-tetrachloro-5,6-dimethoxybenzene
Chemical Name: tetrachloroveratrole
CAS Registry No: 944-61-6
Molecular Formula: C₈H₆Cl₄O₂, C₆Cl₄(OCH₃)₂
Molecular Weight: 275.944
Melting Point (°C):
90 (Lun et al. 1995)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
242.2 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):
Enthalpy of Fusion, ∆Hfus (kJ/mol):
Entropy of Fusion, ∆Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.23 (mp at 90°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.70 (shake flask-GC, Neilson et al. 1984)
1.59 (shake flask-GC/ECD, Lun et al. 1995)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
5.80, 5.90 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)
4.70 (Sarrikoski et al. 1986)
5.90 (Part et al. 1992, quoted, Sangster 1993)
4.86 (shake flask-GC/ECD both phases, Lun et al. 1995)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kbi:
4.40, 4.50 (zebra fish, calculated, Neilson et al. 1984)
Sorption Partition Coefficient, log Koc:
3.45 (sediment, Kp = 2.8 ml·(kg of organic C)-¹, batch sorption equilibrium, Remberger et al. 1986)
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
10.1.3.15 Phenetole

![Chemical Structure of Phenetole](image)

Common Name: Phenetole  
Synonym: ethoxybenzene, ethyl phenyl ether  
Chemical Name: ethoxybenzene, ethyl phenyl ether  
CAS Registry No: 103-73-1  
Molecular Formula: C₈H₁₀O, C₆H₅-O-C₂H₅  
Molecular Weight: 122.164

**Melting Point (°C):**
- 29.52 (Riddick et al. 1986)
- 33.00 (Stephenson & Malanowski 1987)
- 29.43 (Lide 2003)

**Boiling Point (°C):**
- 169.84 (Riddick et al. 1986)
- 172.00 (Stephenson & Malanowski 1987)
- 169.81 (Lide 2003)

**Density (g/cm³ at 20°C):**
- 0.9651, 0.9605 (20°C, 25°C, Dreisbach & Martin 1949; Riddick et al. 1986)

**Molar Volume (cm³/mol):**
- 126.6 (20°C, calculated-density)
- 150.3 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C, F:** 1.0

**Water Solubility (g/m³ or mg/L at 25°C):**
- 1160 (residual volume, Booth & Everson 1948)
- 550 (shake flask-AS, McGowan et al. 1966)
- 569 (shake flask-UV, Vesala 1974)
- 1114 (calculated-K_{ow}, Valvani et al. 1981)
- 1200 (selected, 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):**
- 133.3* (18°C, compiled and evaluated data, temp range 18–172°C, Stull 1947)
- \( \log (P/\text{mmHg}) = 7.40281 – 1808.8/(230 + t/°C) \) (Antoine eq., Dreisbach & Martin 1949)
- 7605* (91.89°C, ebulliometry, measured range 91.89–170°C, Dreisbach & Shrader 1949)
- 20441* (117.43°C, ebulliometry, measured range 117.43–180.608°C, Collerson et al. 1965)
- \( \log (P/\text{mmHg}) = 7.01980 – 1507.267/(194.357 + t/°C) \); temp range 117.43–180.608°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
- \( \log (P/\text{mmHg}) = 6.14658 – 1509.276/(194.648 + t/°C) \), temp range not specified (Antoine eq., Riddick et al. 1986)
Henry’s Law Constant (Pa m³/mol at 25°C): 44.5 (calculated-P/C from selected data)

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

- 2.51 (shake flask, Hansch & Leo 1979; 1987)
- 2.68 (HPLC-\( k' \) correlation, Haky & Young 1984)
- 2.51 (recommended, Sangster 1993)
- 2.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

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

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

Half-Lives in the Environment:

### TABLE 10.1.3.15.1
Reported vapor pressures of phenetole at various temperatures and the coefficients for the vapor pressure equations

| \( \log P = A - B/(T/K) \) | \( \ln P = A - B/(T/K) \) |
| \( \log P = A - B/(C + t/°C) \) | \( \ln P = A - B/(C + t/°C) \) |
| \( \log P = A - B/(T/K) - C \cdot \log (T/K) \) | |

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Collerson et al. 1965</th>
<th>Ambrose et al. 1976</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>summary of literature data</strong></td>
<td>ebulliometry</td>
<td>ebulliometry</td>
<td>comparative ebulliometry</td>
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<tr>
<td>( t/°C )</td>
<td>( P/Pa )</td>
<td>( t/°C )</td>
<td>( P/Pa )</td>
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<tr>
<td>18.1</td>
<td>133.3</td>
<td>91.89</td>
<td>7605</td>
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<td>43.7</td>
<td>666.6</td>
<td>95.6</td>
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<td>56.4</td>
<td>1333</td>
<td>111.56</td>
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<td>70.3</td>
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<td>86.6</td>
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<td>95.4</td>
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<td>108.4</td>
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<td>127.9</td>
<td>26664</td>
<td>157.829</td>
<td>73278</td>
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<td>149.8</td>
<td>53329</td>
<td>157.829</td>
<td>73278</td>
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<td>172</td>
<td>101325</td>
<td>Antoine eq. given by Dreisbach &amp; Martin 1949</td>
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<tr>
<td>( mp/°C )</td>
<td>( –30.2 )</td>
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<tr>
<td>( \text{eq. 2} )</td>
<td>P/mmHg</td>
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<td>B</td>
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<tr>
<td>C</td>
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<tr>
<td>( \text{bp/°C} )</td>
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<td></td>
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<tr>
<td>( \text{mp/°C} )</td>
<td>–29.52</td>
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</tr>
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</table>

(Continued)
TABLE 10.1.3.15.1 (Continued)

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Collerson et al. 1965</th>
<th>Ambrose et al. 1976</th>
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<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
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<td>Antoine eq.</td>
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<td>P/mmHg</td>
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<td>B</td>
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<td>C</td>
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<td>Kirchhoff eq.</td>
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<td>eq. 4</td>
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<td>C</td>
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<tr>
<td>∆H°/(kJ mol⁻¹) = 40.71</td>
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</table>

FIGURE 10.1.3.15.1 Logarithm of vapor pressure versus reciprocal temperature for phenetole.
10.1.3.16 Benzyl ethyl ether

Common Name: Benzyl ethyl ether
Synonym: (ethoxymethyl)benzene, α-ethoxytoluene
Chemical Name: benzyl ethyl ether, (ethoxymethyl)benzene, α-ethoxytoluene
CAS Registry No: 539-30-0
Molecular Formula: C₉H₁₂O, C₆H₅CH₂-O-C₂H₅
Molecular Weight: 136.190
Melting Point (°C):
Boiling Point (°C):
  185.6  (Lide 2003)
Density (g/cm³ at 20°C):
  0.9490  (Weast 1982–83)
  0.9478  (Dean 1985)
Molar Volume (cm³/mol):
  143.5  (20°C, calculated-density)
  172.5  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₜₜ (kJ/mol):
Entropy of Fusion, ΔSₘₜₜ (J/mol K):
Fugacity Ratio at 25°C, 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):
  135*  (calculated-Antoine eq. regression, Stull 1947)
  100  (selected, Riddick et al. 1986)
log (P/kPa) = 6.6496 – 1927.21/(230 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
  135  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.92406 – 2133.29/(–24.38 + T/K); temp range 299–460 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 27.6421 – 3.4249 × 10³/(T/K) – 6.5804·log (T/K) + 9.3417 × 10⁻¹⁰·(T/K) + 1.0547 × 10⁻⁶·(T/K)²;
temp range 309–660 K (vapor pressure eq., Yaws 1994)
95.44*  (25.35°C, transpiration method, measured range 278.3–313.7 K, Krasnykh et al. 2002)
ln (P/Pa) = (305.859/R) – [79968.084/R(T/K)] – (88.80/R)·ln[(T/K)/298.15]; temp range 278–313.7 K (transpiration method, Krasnykh et al. 2002)

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₖₜₜ:
  2.64  (calculated-f const. as per Rekker 1977, Hanai et al. 1981)
  2.16  (Wang et al. 1987)
  2.16  (recommended, Sangster 1993)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₜₑₑ:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
  Air: disappearance t½ < 0.24 h from air for the reaction with OH radical (Darnall et al. 1976).
TABLE 10.1.3.16.1
Reported vapor pressures of benzyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

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

\[
\log \left( \frac{P}{\text{mmHg}} \right) = A - B/(C + t/°C) \quad (2) \quad \ln \frac{P}{\text{mmHg}} = A - B/(C + t/°C) \quad (2a)
\]

\[
\log \left( \frac{P}{\text{Pa}} \right) = A - B/(C + T/K) \quad (3)
\]

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

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
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Stull 1947
Krasnykh et al. 2002

FIGURE 10.1.3.16.1 Logarithm of vapor pressure versus reciprocal temperature for benzyl ethyl ether.
10.1.3.17 Styrene oxide

Common Name: Styrene oxide
Synonym: (1,2-epoxyethyl)benzene, phenylepoxyethane
Chemical Name: (1,2-epoxyethyl)benzene, phenylepoxyethane, styrene oxide
CAS Registry No: 96-09-3
Molecular Formula: C₈H₈O
Molecular Weight: 120.149
Melting Point (°C):
-35.6 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
194.1 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
1.0523 (16°C, Weast 1982–83; Dean 1985)
1.0500 (Verschueren 1983)
Molar Volume (cm³/mol):
114.4 (20°C, calculated-density)
136.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
2800 (quoted, Verschueren 1983)
3020; 4570 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
Vapor Pressure (Pa at 25°C):
40.0 (Verschueren 1983)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
1.84 (shake flask-HPLC, Pratesi et al. 1979)
1.51 (shake flask-GC, Serrentino et al. 1983)
1.61 (shake flask, Log P Database, Hansch & Leo 1987)
1.43 (Deneer et al. 1988)
1.61 (recommended, Sangster 1989, 1993)
1.51 (pH 7.5, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{½}:
Volatilization:
Photolysis: t_{½} = 12.3–123 h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: rate constants k = (434 ± 12) × 10^{-8} s^{-1} at pH 7.25 and k = (1690 ± 620) × 10^{-8} s^{-1} at pH 7.3 in sediment pores both at 25°C for water containing 0.1% w/w CH₂O as sterilant with 1-phenyl-1,2-ethanediol as major hydrolyzed product (Haag & Mill 1988);
t_{1/2} = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C, the hydrolysis half-lives at pH 5, 7 and 9 are 0.00385, 21.4 and 27.5 h (Haag & Mill 1988; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic t_{1/2} = 24–168 h, based on biological screening test data (Schmidt-Bleek et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic t_{1/2} = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:
Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: disappearance t_{1/2} < 0.24 h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);

\[ t_{1/2} = 12.3–123 \text{ h}, \text{ based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).} \]

Surface water: t_{1/2} = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Ground water: t_{1/2} = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Sediment:
Soil: t_{1/2} = 0.00385–27.5 h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).
10.1.3.18 Diphenyl ether

![Chemical structure of Diphenyl ether]

**Common Name:** Diphenyl ether  
**Synonym:** phenyl ether, diphenyl oxide, phenyl ether, 1,1′-oxybisbenzene, phenoxybenzene 
**Chemical Name:** diphenyl ether, diphenyloxide, phenoxybenzene 
**CAS Registry No:** 101-84-8 
**Molecular Formula:** C₁₂H₁₀O, (C₆H₅)₂O  
**Molecular Weight:** 170.206 

**Melting Point (°C):**  
26.87 (Lide 2003) 
**Boiling Point (°C):**  
258 (Lide 2003) 

**Density (g/cm³ at 20°C):**  
1.0748 (Weast 1982–83) 

**Molar Volume (cm³/mol):**  
158.6 (20°C, calculated-density) 
166.6 (Ruelle & Kesselring 1997) 
195.6 (calculated-Le Bas method at normal boiling point) 

**Enthalpy of Fusion, ΔH_fus (kJ/mol):**  
17.217 (quoted, Riddick et al. 1986) 
16.16 (Ruelle & Kesselring 1997) 

**Entropy of Fusion, ΔS_fus (J/mol K):**  
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.923 (mp 28.5°C) 

**Water Solubility (g/m³ or mg/L at 25°C):**  
4000 (shake flask-residue-volume, Booth & Everson 1948) 
18.7 (shake flask-UV, Vesala 1974) 
18.0 (shake flask-HPLC, Banerjee et al. 1980; Pearlman et al. 1984) 
21.0 (Verschueren 1983) 
18.3900 (quoted values, Riddick et al. 1986) 
46.88 (supercooled liquid S₁, RP-HPLC-RI correlation, Kurz & Ballschmiter 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):**  
133.3* (66.1°C, summary of literature data, temp range 66.1–258.5°C, Stull 1947) 
10.01* (40°C, dynamic method, measured range 40–60°C, Bent & Francel 1948) 

\[
\log (P/\text{mmHg}) = 9.6842 - 3351.9/(t/°C + 273.1); \text{measured range 40–60°C (dynamic method-gas saturation, Bent & Francel 1948)} 
\]
\[
\log (P/\text{mmHg}) = 7.65339 - 2328.0/(2325.5/(T/K) + 3.92657\log (T/K); \text{temp range 204.2–270.9°C (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)} 
\]
\[
\log (P/\text{mmHg}) = 19.48322 - 2328.0/(T/K) - 3.92657\log (T/K); \text{temp range 204.2–270.9°C (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)} 
\]
\[
\log (P/\text{mmHg}) = [-0.2185 \times 12325.5/(T/K)] + 7.955679; \text{temp range 66.1–258.5°C (Antoine eq., Dreisbach & Martin 1949)} 
\]
\[
\log (P/kPa) = 6.13913 - 1802.984/(T/K) - 95.013; \text{temp range 477–544 K (Antoine eq., Ambrose et al. 1976)} 
\]
\[
2.67 (Verschueren 1983) 
\]
\[
1.82 (calculated-Antoine eq., Boublik et al. 1984) 
\]
\[
\log (P/kPa) = 7.01104 - 1799.712/(177.744 + t/°C); \text{temp range 204–270°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} 
\]
log (P/kPa) = 6.13606 – 1799.811/(177.756 + t°C); temp range 204.2–271°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 7.01104 – 1799.71/(177.74 + t°C); temp range: 204–271°C (Antoine eq., Dean 1985, 1992)
2.84 (selected, Riddick et al. 1986)
log (P/kPa) = 6.13913 – 1902.984/(178.137 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
2.93 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 8.7109 – 3351.9/(T/K); temp range 313–333K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = –26.9635 – 2.5909 × 10³/(T/K) + 16.42·log (T/K) – 2.4334 × 10⁻²·(T/K) + 1.0244 × 10⁻⁵·(T/K)²; temp range 300–763 K (vapor pressure eq., Yaws 1994)
2.40 (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry’s Law Constant (Pa m³/mol at 25°C):
25.1 (calculated-P/C using selected data)
8.71 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
4.21, 4.36 (shake flask values, Leo et al. 1971)
4.20 (shake flask-GC, Chiou et al. 1977)
4.25 (calculated-fragment const., Rekker 1977)
4.26 (Hansch & Leo 1979)
4.08 (shake flask-HPLC, Banerjee et al. 1980)
3.79 (estimated-HPLC/MS correlation, Burkhard et al. 1985)
4.24 (calculated-f const., Burkhard et al. 1985)
3.87 (HPLC-RT correlation, Eadsforth 1986)
4.28 (shake flask, Log P Database, Hansch & Leo 1987)
4.21 (recommended, Sangster 1989, 1993)
3.949, 4.014 (shake flask method, Brooke et al. 1990)
4.21 (recommended, Hansch et al. 1995)
3.97 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
6.42 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF:
2.29 (rainbow trout, calculated, Veith et al. 1979)
2.29; 2.89 (quoted exptl., calculated-K_{OW}/K_{AW}, Mackay 1982)

Sorption Partition Coefficient, log K_{OC}:
3.29; 3.41 (soil, quoted exptl.; calculated-MCI χ, Meylan et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, t_½:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
k_1 = 5.5 h⁻¹, k_2 = 0.0275 h⁻¹ (trout, Hawker & Connell 1985)
1/k_2 = 36 h (trout, Hawker & Connell 1988)
k_2 = 0.676 h⁻¹ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:
Air: disappearance t_½ < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).
TABLE 10.1.3.18.1

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

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

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**∆H_v = 64.02 kJ/mol**

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**Dreisbach & Shrader 1949**

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**Antoine eq. given by Dreisbach & Martin 1949**

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**∆H_v = 48.62 kJ/mol**
FIGURE 10.1.3.18.1 Logarithm of vapor pressure versus reciprocal temperature for diphenyl ether.
10.1.4 POLYCHLORINATED DIPHENYL ETHERS (PCDES)

10.1.4.1 2-Chlorodiphenyl ether (PCDE-1)

Common Name: 2-Chlorodiphenyl ether
Synonym: 2-CDPE, PCDE-1, 2-chlorobiphenyl ether
Chemical Name: 2-chlorodiphenyl ether
CAS Registry No: 2689-07-8
Molecular Formula: C_{12}H_{9}ClO
Molecular Weight: 204.652
Melting Point (°C):
  45  (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  216.5  (calculated-Le Bas method at normal boiling point)
  179.5  (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.634 (mp at 45°C)
Water Solubility (g/m³ or mg/L at 25°C):
  3.40; 4.80  (quoted exptl.; calculated-molar volume and MP, Ruelle & Kesselring 1997)
  3.40  (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
  0.537  (P_{L}, GC-RI correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol):
  32.36  (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{OW}:
  4.45  (HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{OA}:
  6.33  (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{Bi}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Photolysis: photolysis rate k_{p} = 0.0035 d⁻¹ with a half-life of 200 d in summer sunlight; k_{p}(exptl) = 3.4 × 10⁻⁸ s⁻¹ with t_{1/2} = 240 h, k_{p}(calc) = 3.1 × 10⁻⁹ s⁻¹ in winter sunlight, at 40° L in surface waters (Dulin et al. 1986)
Half-Lives in the Environment:
Air:
Surface water: photolysis t_{1/2} = 200 d in summer sunlight and t_{1/2} = 240 d in winter sunlight at 40° L in surface waters (Dulin et al. 1986)
Ground water:
Sediment:
Soil:
Biota: t_{1/2} = 4–63 d in trout Cl_{1}-DPEs to Cl_{4}-DPEs (Niimi et al. 1994).
10.1.4.2 4-Chlorodiphenyl ether

Common Name: 4-Chlorodiphenyl ether
Synonym: 4-chlorophenyl phenyl ether, 1-chloro-4-phenoxybenzene, p-chlorophenyl phenyl ether, 4-chlorodiphenyl ether, monochlorodiphenyl oxide
Chemical Name: 4-chlorophenyl phenyl ether, 4-chlorodiphenyl ether
CAS Registry No: 7005-72-3
Molecular Formula: C₁₂H₉ClO
Molecular Weight: 204.652

Melting Point (°C):
-6.0 (Callahan et al. 1979)
-8.0 (Mabey et al. 1982)

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

Density (g/cm³ at 20°C):
1.2026 (15°C, Weast 1982–83; Lide 2003)

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

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

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

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
3.30 (Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)
59.04 (Isnard & Lambert 1988, 1989)

Vapor Pressure (Pa at 25°C):
0.360 (calculated, Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
22.19 (calculated-P/C, Mabey et al. 1982)
22.29 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
4.08 (Branson 1977; quoted, Callahan et al. 1979; Ryan et al. 1988; Isnard & Lambert 1988, 1989)
5.079 (calculated, Mabey et al. 1982)

Bioconcentration Factor, log BCF:
2.867 (rainbow trout muscle, Branson 1977; quoted, Callahan et al. 1979)
4.255 (microorganisms-water, calculated-$K_{\text{OW}}$, Mabey et al. 1982)
2.87 (quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, log $K_{\text{OC}}$:
4.763 (sediment-water, calculated-$K_{\text{OW}}$, Mabey et al. 1982)

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

Volatileization:
Photolysis: photolysis rate $k_p = 0.19$ d⁻¹ with $t_{\frac{1}{2}} = 3.6$ d in summer sunlight; $k_p(\text{exptl}) < 2.0 \times 10^{-8}$ s⁻¹ with $t_{\frac{1}{2}} > 400$ h, $k_p(\text{calc}) = 3.7 \times 10^{-8}$ s⁻¹ in winter sunlight, both at 40° L in surface waters (Dulin et al. 1986)
Oxidation: $k << 360$ M⁻¹ h⁻¹ for singlet oxygen and $k << 1.0$ M⁻¹ h⁻¹ for peroxy radical (Mabey et al. 1982)

Hydrolysis:
Biodegradation: $t_{1/2} = 4.0 \text{ h}$, measured only in activated sludge (Branson 1978; quoted, Callahan et al. 1979).

Biotransformation: estimated rate constant $k = 1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Surface water: photolysis $t_{1/2} = 3.6 \text{ d}$ summer sunlight and $t_{1/2} > 400 \text{ d}$ in winter sunlight at $40^\circ \text{ L}$ surface waters (Dulin et al. 1986)
10.1.4.3 2,4-Dichlorodiphenyl ether (PCDE-8)

Common Name: 2,4-Dichlorodiphenyl ether
Synonym: 2,4-DCDPE, PCDE-8
Chemical Name:
CAS Registry No: 51892-26-3
Molecular Formula: C₁₂H₈Cl₂O
Molecular Weight: 239.097
Melting Point (°C): 
Boiling Point (°C): 
Density (g/cm³): 
Molar Volume (cm³/mol):
237.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), \(F\):
Water Solubility (g/m³ or mg/L at 25°C):
5.605 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
0.123 (\(P_L\), GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
5.25 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
5.62 (Oliver & Niimi 1984)
4.93 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):
7.60 (calculated-\(K_{\text{ow}}/K_{\text{aw}}\), Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log \(K_B\):
3.97 (rainbow trout, Oliver & Niimi 1984)
Sorption Partition Coefficient, log \(K_{\text{oc}}\):
Environmental Fate Rate Constant, \(k\), and Half-Lives, \(t_\text{1/2}\):
Half-Lives in the Environment:
Biota: \(t_{1/2} = 3–63\) d for Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).
10.1.4.4 2,6-Dichlorodiphenyl ether (PCDE-10)

Common Name: 2,6-Dichlorodiphenyl ether  
Synonym: 2,6-DCDPE, PCDE-10  
Chemical Name:  
CAS Registry No: 28419-69-4  
Molecular Formula: C₁₂H₈Cl₂O  
Molecular Weight: 239.097  
Melting Point (°C): 39 (Ruelle & Kesselring 1997)  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
237.4 (calculated-Le Bas method at normal boiling point)  
192.4 (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, ΔHₚₑₙ (kJ/mol):  
Entropy of Fusion, ΔSₚₑₙ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₚₑₙ = 56 J/mol K), F: 0.729 (mp at 39°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
2.08; 0.213 (quoted expl., calculated-molar volume and mp, Ruelle & Kesselring 1997)  
2.08 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
Vapor Pressure (Pa at 25°C):  
0.174 (supercooled liquid Pₜ, GC-RI correlation, Kurz & Kesselring 1997)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
19.95 (calculated-P/C, Kurz & Kesselring 1997)  
Octanol/Water Partition Coefficient, log Kₜₔₜₕ:  
4.64 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
Octanol/Air Partition Coefficient, log Kₐₕₕ:  
6.73 (calculated-Kₜₔₜₕ/Kₐₕₕ, Kurz & Ballschmiter 1999)  
Bioconcentration Factor, log BCF or log K₉ₕ:  
Sorption Partition Coefficient, log Kₜₕₜₚ:  
Environmental Fate Rate Constants, k, and Half-Lives, tₜₕ:  
Half-Lives in the Environment:  
Biota: tₜₕ = 4–63 d Clₙ-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).
10.1.4.5 2,4,4′-Trichlorodiphenyl ether (PCDE-28)

![Chemical Structure](image)

Common Name: 2,4,4′-Trichlorodiphenyl ether
Synonym: 2,4,4′-TCDPE, PCDE-28
Chemical Name: 2,4,4′-trichlorodiphenyl ether
CAS Registry No: 59030-21-3
Molecular Formula: C₁₂H₇Cl₃O
Molecular Weight: 273.543
Melting Point (°C):
- oil (Navalainen et al. 1994)
- 40 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
- 258.3 (calculated-Le Bas method at normal boiling point)
- 205.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHₚₑₜ (kJ/mol):
Entropy of Fusion, ΔSₚₑₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₑₜ = 56 J/mol K), F: 0.712 (mp at 40°C)
Water Solubility (g/m³ or mg/L at 25°C):
- 0.102; 0.0385 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)
- 0.101 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
- 0.0204 (supercooled liquid P_L, GC-RI correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol):
- 33.88 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{ow}:
- 5.53 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{oa}:
- 7.19 (calculated-K_{ow}/K_{aw}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{b}:
- 2.98; 3.36 (concn of 2,4,4′-trichloro-DPE 39.3; 118 µg/L, juvenile Atlantic salmon, 96-h exposure, Zitko & Carson 1977)
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
- Biota: excretion t_{ex} = 235 h following uptake from water, excretion t_{ex} = 15 d following uptake from food for juvenile salmon (Zitko & Carson 1977);
- average t_{ex} = 15 d in salmon for trichloro-DPE congeners; biological t_{ex} = 63 d (range 46–104 d) in rainbow trout (average value for trichlorodiphenyl ethers (Niimi 1986);
- t_{ex} = 4–63 d Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).
10.1.4.6 2,4,5-Trichlorodiphenyl ether (PCDE-29)

Common Name: 2,4,5-Trichlorodiphenyl ether
Synonym: 2,4,5-TCDPE, PCDE-29
Chemical Name: 2,4,5-trichlorodiphenyl ether
CAS Registry No: 52322-80-2
Molecular Formula: C₁₂H₇Cl₃O
Molecular Weight: 273.543
Melting Point (°C):
- oil (Opperhuizen & Voors 1987) 61
- 61 (Ruelle & Kesselring 1997)
Boiling Point (°C): 
Density (g/cm³):
Molar Volume (cm³/mol):
- 258.3 (calculated-Le Bas method at normal boiling point)
- 205.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol): 
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F: 0.443 (mp at 61°C)
Water Solubility (g/m³ or mg/L at 25°C):
- 0.050 (Opperhuizen 1986)
- 0.072; 0.0486 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
- 0.072 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
- 0.0288 (Pₐ, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol):
- 112.2 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log Kₗₜₜ:
- 5.0 (estimated, Opperhuizen 1986)
- 5.44 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)
- 5.58 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log Kₐₜ:
- 6.92 (calculated-Kₗₜₜ/Kₐₜ, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K₉ₐ:
- 4.18 (guppy, 8-d exposure, Opperhuizen & Voors 1987)
Sorption Partition Coefficient, log K₉ₜ:
Environmental Fate Rate Constants, k, and Half-Lives, tᵢ:
Biotransformation: rate of metabolism k = 0.27 d⁻¹ (guppy, 8-d exposure, Opperhuizen & Voors 1987)
Bioconcentration and Uptake and Elimination Rate Constants (kᵢ and kₑ):
- kᵢ > 5 × 10² d⁻¹ (guppy, Opperhuizen 1986)
- kₑ = 1.5 × 10³ mL g⁻¹ d⁻¹ (guppy, 8-d exposure, Opperhuizen & Voors 1987)
- kₑ = 0.34 d⁻¹ (guppy, elimination period 56 d, Opperhuizen & Voors 1987)
Half-Lives in the Environment:

Biota: average excretion $t_{1/2} = 15$ d for trichloro-DPE congeners in salmon; biological $t_{1/2} = 63$ d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);

$t_{1/2} = 4$–$63$ d for Cl$_1$-DPEs to Cl$_4$-DPEs in trout (Niimi et al. 1994).
10.1.4.7 2,4′,5-Trichlorodiphenyl ether (PCDE-31)

Common Name: 2,4′,5-Trichlorodiphenyl ether
Synonym: 2,4′,5-TCDPE, PCDE-31
Chemical Name: 2,4′,5-trichlorodiphenyl ether
CAS Registry No: 65075-00-5
Molecular Formula: C₁₂H₇Cl₃O
Molecular Weight: 273.543
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
258.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Enterropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
0.0993  (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.0229  (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C):
6.31  (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_OW:
5.66  (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
5.70  (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_OA:
8.25  (calculated-K_OW/K_AW, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:
3.30; 2.93 (ave. concn of 2,4′,5-trichloro-DPE 2.37; 7.01 µg/L, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, log K_OC:

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

Half-Lives in the Environment:
Biota: excretion t₁₀ = 310 h following uptake from water; t₁₀ = 26 d following uptake from food for juvenile Atlantic salmon (Zitko & Carson 1976);
average excretion t₅ = 15 d for trichloro-DPE congeners in salmon; biological t₁₀ = 63 d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);
t₅ = 4–63 d Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).
10.1.4.8 2,2′,4,4′-Tetrachlorodiphenyl ether (PCDE-47)

Common Name: 2,2′,4,4′-Tetrachlorodiphenyl ether
Synonym: 2,2′,4,4′-TCDPE, PCDE-47, 2,2′,4,4′-tetrachlorobiphenyl ether, 2,2′,4,4′-TCBP
Chemical Name: 2,2′,4,4′-tetrachlorodiphenyl ether
CAS Registry No: 28076-73-5
Molecular Formula: C₁₂H₆Cl₄O
Molecular Weight: 307.988

Melting Point (°C):
69–70 (Navalainen et al. 1994)
69 (Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
279.2 (calculated-Le Bas method at normal boiling point)
218.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_fus (kJ/mol):

Entropy of Fusion, ΔS_fus (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.366 (mp at 69.5°C)

Water Solubility (g/m³ or mg/L at 25°C):
0.0466; 0.0154 (quoted exp. , calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.0466 (supercooled liquid, RP-HPLC-RI, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
0.00525 (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C):
34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
5.95 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{AO}:
7.80 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
Biota: average excretion t₁/₂ = 55 d in salmon for tetrachloro-DPE congeners; mean biological t₁/₂ = 119 d (range 82–213 d) in rainbow trout (Niimi 1986);
t₁/₂ = 4–63 d for Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).
10.1.4.9 2,3′,4,4′-Tetrachlorodiphenyl ether (PCDE-66)

Common Name: 2,3′,4,4′-Tetrachlorodiphenyl ether
Synonym: 2,3′,4,4′-DCPE, PCDE-66
Chemical Name: 2,3′,4,4′-tetrachlorodiphenyl ether
CAS Registry No: 61328-46-9
Molecular Formula: C_{12}H_{6}Cl_{4}O
Molecular Weight: 307.988
Melting Point (°C):
  oil (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  279.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  0.0308 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
  0.00407 (supercooled liquid P_{L}, GC-RI correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  40.74 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{OW}:
  6.13 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{AO}:
  7.91 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{B}:
  3.43; 3.01 (ave. concn of 2,3′,4,4′-tetrachloro-DPE 2.07; 6.03 µg/L, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
  Biota: excretion t_{1/2} = 370 h following uptake from water, t_{1/2} = 55 d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);
  average excretion t_{1/2} = 55 d in salmon for tetrachloro-DPE congeners; mean biological t_{1/2} = 119 d (range 82–213 d) in rainbow trout (Niimi 1986);
  t_{1/2} = 4–63 d in trout for Cl_{1}-DPEs to Cl_{4}-DPEs (Niimi et al. 1994).
10.1.4.10 2,4,4',5-Tetrachlorodiphenyl ether (PCDE-74)

Common Name: 2,4,4',5-Tetrachlorodiphenyl ether
Synonym: 2,4,4',5-PCDE, PCDE-74
Chemical Name: 2,4,4',5-tetrachlorodiphenyl ether
CAS Registry No: 61328-45-8
Molecular Formula: C_{12}H_{6}Cl_{4}O
Molecular Weight: 307.988
Melting Point (°C): 62–63 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
279.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.0281 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
4.79 × 10⁻³ (P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
52.48 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{OW}:
5.99 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{OA}:
7.66 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Biota: average t_{1/2} = 55 d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986); mean biological t_{1/2} = 108 d (range 62–407 d) in rainbow trout (Niimi 1986);
t_{1/2} = 4–63 d in trout for Cl_{1}-DPEs to Cl_{4}-DPEs; t_{1/2} = 15 d for Cl_{3}-DPE to Cl_{4}-DPE in waterborne exposed salmon and t_{1/2} = 55 d for diet-exposed fish (Niimi et al. 1994).
**10.1.4.11 3,3′,4,4′-Tetrachlorodiphenyl ether (PCDE-77)**

![Structure of 3,3′,4,4′-Tetrachlorodiphenyl ether]

**Common Name:** 3,3′,4,4′-Tetrachlorodiphenyl ether  
**Synonym:** 3,3′,4,4′-PCDE, PCDE-77  
**Chemical Name:** 3,3′,4,4′-tetrachlorodiphenyl ether  
**CAS Registry No:** 56348-72-2  
**Molecular Formula:** C₁₂H₆Cl₄O  
**Molecular Weight:** 307.988  
**Melting Point (°C):**  
   - 69–71 (Navalainen et al. 1994)  
   - 70 (Ruelle & Kesselring 1997)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):**  
   - 279.2 (calculated-Le Bas method at normal boiling point)  
   - 218.2 (Ruelle & Kesselring 1997)  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**  
**Entropy of Fusion, ΔS_{fus} (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.362 (mp at 70°C)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
   - 0.020 (Opperhuizen 1986)  
   - 0.0323; 0.00991; (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)  
   - 0.0323 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
**Vapor Pressure (Pa at 25°C):**  
   - 2.57 × 10⁻³ (P_L, GC-RI correlation, Kurz & Ballschmiter 1999)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
**Octanol/Water Partition Coefficient, log K_{ow}:**  
   - 6.0 (estimated, Opperhuizen 1986)  
   - 5.78 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)  
   - 6.36 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
**Octanol/Air Partition Coefficient, log K_{oa}:**  
   - 8.36 (calculated-K_{ow}/K_{aw}, Kurz & Ballschmiter 1999)  
**Bioconcentration Factor, log BCF or log K_{b}:**  
   - 4.50 (guppy, 8-d exposure, Opperhuizen & Voors 1987)  
   - 4.51; 4.09 (guppy; trout muscle, Niimi et al. 1994)  
   - 4.46–4.99 (calculated-K_{ow}, Niimi et al. 1994)  
**Sorption Partition Coefficient, log K_{oc}:**

**Environmental Fate Rate Constants, k, and Half-Lives, tₜ:**  
- Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):  
   - k₁ > 5 × 10² d⁻¹ (Guppy, Opperhuizen 1986)
$k_1 = 9.6 \times 10^2 \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, 8-d exposure, Opperhuizen & Voors 1987)

$k_2 = 0.03 \text{ d}^{-1}$ (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986)

mean biological $t_{1/2} = 134$ d (range 73–792 d) in rainbow trout (Niimi 1986);

t$_{1/2} = 23$ d in guppy, $t_{1/2} = 29$ d in trout muscle (Niimi et al. 1994).
10.1.4.12 2,2',3,4,4'-Pentachlorodiphenyl ether (PCDE-85)

Common Name: 2,2’,3,4,4’-Pentachlorodiphenyl ether
Synonym: PDCE-85
Chemical Name: 2,2’,3,4,4’-pentachlorodiphenyl ether
CAS Registry No: 71585-37-0
Molecular Formula: C_{12}H_{5}Cl_{5}O
Molecular Weight: 342.433
Melting Point (°C):
65–67 (Navalainen et al. 1994)
66 (Ruelle & Kesselring 1997)
Boiling Point (°C):

Density (g/cm³):
Molar Volume (cm³/mol):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.396 (mp at 66°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.0124; 0.00609 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
0.0124 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
6.92 × 10⁻⁴ (supercooled liquid P_L, GC-RI correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol):
19.05 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{OW}:
6.28 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{OA}:
8.39 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Biota: average $t_\text{i} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986)
biological $t_\text{i} \sim 113$ d (range 81–144 d, average value for pentachloro-DPE congeners, Niimi 1986);
$t_\text{i} = 15$ d for Cl₂-DPE to Cl₅-DPE in waterborne exposed salmon and $t_\text{i} = 55$ d for diet-exposed fish (Niimi et al. 1994).
10.1.4.13 2,2',4,4',5-Pentachlorodiphenyl ether (PCDE-99)

Common Name: 2,2',4,4',5-Pentachlorodiphenyl ether
Synonym: 2,2',4,4',5-PCDE, PCDE-99
Chemical Name: 2,2',4,4',5-pentachlorodiphenyl ether
CAS Registry No: 60123-64-0
Molecular Formula: C_{12}H_5Cl_5O
Molecular Weight: 342.433

Melting Point (°C):
- oil (Navalainen et al. 1994)
- 25 (Passivirta et al. 1999)

Boiling Point (°C):
- Density (g/cm³):
  - 300.1 (calculated-Le Bas method at normal boiling point)
  - 231.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
- Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 1.0
  - 1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
- $5.06 \times 10^{-3}$; $0.0153$ (quoted exp., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- $8.406 \times 10^{-3}$ (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- $\log [S_l/(mol/L)] = -1.392 - 866.2/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- $1.35 \times 10^{-3}$ (P₁, GC-RT correlation, Kurz & Ballschmiter 1999)
- $1.34 \times 10^{-3}$; $1.34 \times 10^{-3}$ (liquid P₁, GC-RT correlation; converted to solid P₄ with fugacity ratio F, Passivirta et al. 1999)
- $\log (P_l/Pa) = 11.90 - 4404/(T/K)$ (solid, Passivirta et al. 1999)
- $\log (P_l/Pa) = 8.95 - 3525/(T/K)$ (liquid, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- $54.95$ (calculated-P/C, Kurz & Ballschmiter 1999)
- $\log [H/(Pa m³/mol)] = 10.34 - 2659/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:
- $6.38$ (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- $7.46, 7.20$ (quoted lit., calculated from lit. $\log K_{\text{ow}}$ and estimated $\log S_l$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{oa}}$:
- $8.03$ (calculated-$K_{\text{ow}}/K_{\text{aw}}$, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log $K_{\text{b}}$:
- $3.15; 2.77$ (4.01; 12.0 µg/L, ave. concn of 2,2',4,4',5-PCDPE (reported as 2,2',4,5-TCDPE), juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

- Biota: excretion $t_\text{½} = 370$ h following uptake from water, $t_\text{½} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);
- average excretion $t_{\text{½}} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{\text{½}} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);
- $t_{\text{½}} = 15$ d for Cl$_4$-DPE to Cl$_5$-DPE in waterborne exposed salmon and $t_{\text{½}} = 55$ d for diet-exposed fish (Niimi et al. 1994).
10.1.4.14 2,2',4,4',6-Pentachlorodiphenyl ether (PCDE-100)

Common Name: 2,2',4,4',6-Pentachlorodiphenyl ether
Synonym: 2,2',4,4',6-PCDE, PCDE-100
Chemical Name: 2,2',4,4',6-pentachlorodiphenyl ether
CAS Registry No: 104294-16-8
Molecular Formula: C_{12}H_{5}Cl_{5}O
Molecular Weight: 342.433
Melting Point (°C):
45–46 (Navalainen et al. 1994)
46 (Passivirta et al. 1999)
Boiling Point (°C): 45 (Passivirta et al. 1999)
Density (g/cm³):
300.1 (calculated-Le Bas method at normal boiling point)
231.1 (Passivirta et al. 1999)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
56.5 (calculated, Passivirta et al. 1999)
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 and reported temperature dependence equations):
0.0160 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
\[ \log [S_L/(mol/L)] = -1.392 - 943.0/(T/K) \] (liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.19 \times 10^{-3} (supercooled liquid \( P_L \), GC-RT correlation, Kurz & Ballschmiter 1999)
2.17 \times 10^{-3}, 1.34 \times 10^{-3} (liquid \( P_L \), GC-RT correlation; converted to solid \( P_S \) with fugacity ratio F, Passivirta et al. 1999)
\[ \log (P_L/Pa) = 11.90 - 4408/(T/K) \] (solid, Passivirta et al. 1999)
\[ \log (P_S/Pa) = 8.95 - 3467/(T/K) \] (liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
46.77 (calculated-P/C, Kurz & Ballschmiter 1999)
\[ \log [H/(Pa·m³/mol)] = 10.34 - 2524/(T/K) \] (Passivirta et al. 1999)
Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
6.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
7.11, 6.31 (quoted lit., calculated from lit. \( \log K_{\text{OW}} \) and estimated \( \log S_L \), Passivirta et al. 1999)
Octanol/Air Partition Coefficient, \( \log K_{\text{OA}} \):
7.83 (calculated-\( K_{\text{OW}}/K_{\text{AW}} \), Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log $K_B$;
Sorption Partition Coefficient, log $K_{OC}$;
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$;

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);
average excretion $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{1/2} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);
$t_{1/2} = 15$ d for Cl$_2$-DPE to Cl$_5$-DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).
10.1.4.15 2,2’,4,5,5’-Pentachlorodiphenyl ether (PCDE-101)

Common Name: 2,2’,4,5,5’-Pentachlorodiphenyl ether  
Synonym: PDCE-101  
Chemical Name: 2,2’,4,5,5’-pentachlorodiphenyl ether  
CAS Registry No: 131138-21-1  
Molecular Formula: C\textsubscript{12}H\textsubscript{5}Cl\textsubscript{5}O  
Molecular Weight: 342.433  
Melting Point (°C): oil (Navalainen et al. 1994)  
Boiling Point (°C):  
Density (g/cm\textsuperscript{3}):  
Molar Volume (cm\textsuperscript{3}/mol): 300.1 (calculated-Le Bas method at normal boiling point)  
231.1 (Ruelle & Kesselring 1997)  
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):  
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):  
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F: 1.0  
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C): 0.00943; 0.0153 (quoted exper.; calculated-molar volume and mp, Ruelle & Kesselring 1997)  
0.00943 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
Vapor Pressure (Pa at 25°C): 1.74 × 10\textsuperscript{-3} (supercooled liquid P\textsubscript{L}, GC-RT correlation, Kurz & Ballschmiter 1999)  
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol): 63.10 (calculated-P/C, Kurz & Ballschmiter 1999)  
Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\): 6.22 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)  
Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\): 7.81 (calculated-\(K_{\text{OW}}/K_{\text{AW}}\), Kurz & Ballschmiter 1999)  
Bioconcentration Factor, log BCF or log \(K_{B}\):  
Sorption Partition Coefficient, log \(K_{OC}\):  
Environmental Fate Rate Constants, k, and Half-Lives, \(t_{1/2}\):  
Half-Lives in the Environment:  
Biota: excretion \(t_{1/2} = 370\) d following uptake from water; \(t_{1/2} = 55\) d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);  
average \(t_{1/2} = 55\) d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986);  
biological \(t_{1/2} = 113\) d (range 81–144 d) in rainbow trout (average value of pentachloro-DPE, Niimi 1986);  
\(t_{1/2} = 15\) d for Cl\textsubscript{4}-DPE to Cl\textsubscript{5}-DPE in waterborne exposed salmon and \(t_{1/2} = 55\) d for diet-exposed fish (Niimi et al. 1994).
10.1.4.16 2,3,3’,4,4’-Pentachlorodiphenyl ether (PCDE-105)

Common Name: 2,3,3’,4,4’-Pentachlorodiphenyl ether
Synonym: PCDE-105
Chemical Name: 2,3,3’,4,4’-pentachlorodiphenyl ether
CAS Registry No: 85918-31-6
Molecular Formula: C_{12}H_{5}Cl_{5}O
Molecular Weight: 324.433
Melting Point (°C):
   64–66 (Navalainen et al. 1994)
   65 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   300.1 (calculated-Le Bas method at normal boiling point)
   231.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \, \text{J/mol K} \)), F: 0.405 (mp at 65°C)
Water Solubility (g/m³ or mg/L at 25°C):
   0.00732; 0.0059 (quoted exp., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
   0.00732 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
   5.13 \times 10^{-4} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa-m³/mol at 25°C):
   23.99 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
   6.51 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):
   8.52 (calculated-\( K_{\text{ow}}/K_{\text{aw}} \), Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log \( K_{\text{b}} \):
Sorption Partition Coefficient, log \( K_{\text{oc}} \):
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{\frac{1}{2}} \):
Half-Lives in the Environment:
   Biota: average \( t_{\frac{1}{2}} = 55 \, \text{d} \) in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)
   biological \( t_{\frac{1}{2}} \sim 113 \, \text{d} \) (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);
   \( t_{\frac{1}{2}} = 15 \, \text{d} \) for Cl₃-DPE to Cl₅-DPE in waterborne exposed salmon and \( t_{\frac{1}{2}} = 55 \, \text{d} \) for diet-exposed fish (Niimi et al. 1994).
10.1.4.17 3,3',4,4',5-Pentachlorodiphenyl ether (PCDE-126)

Common Name: 3,3',4,4',5-Pentachlorodiphenyl ether
Synonym: PCDE-126
Chemical Name: 3,3',4,4',5-pentachlorodiphenyl ether
CAS Registry No: 94339-59-0
Molecular Formula: C₁₂H₅Cl₅O
Molecular Weight: 342.433
Melting Point (°C):
   68–70 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   300.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   1.93 × 10⁻³ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
   5.62 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
   100 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
   6.83 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
   6.88 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
   8.22 (calculated-\( K_{\text{OW}}/K_{\text{AW}} \), Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log \( K_B \):
Sorption Partition Coefficient, log \( K_{\text{OC}} \):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
Half-Lives in the Environment:
   Biota: average \( t_{1/2} = 55 \) d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)
   biological \( t_{1/2} \sim 113 \) d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);
   \( t_{1/2} = 15 \) d for Cl₄-DPE to Cl₅-DPE in waterborne exposed salmon and \( t_{1/2} = 55 \) d for diet-exposed fish (Niimi et al. 1994).
10.1.4.18 2,2’,3,3’,4,4’-Hexachlorodiphenyl ether (PCDE-128)

![Chemical Structure](image)

Common Name: 2,2’,3,3’,4,4’-Hexachlorodiphenyl ether
Synonym: PCDE-128
Chemical Name: 2,2’,3,3’,4,4’-hexachlorodiphenyl ether
CAS Registry No: 71585-39-2
Molecular Formula: C_{12}H_4Cl_6O
Molecular Weight: 376.878

Melting Point (°C):
- 141–142 (Navalainen et al. 1994)
- 95 (Ruelle & Kesselring 1997)

Boiling Point (°C):
- 141–142 (Navalainen et al. 1994)
- 95 (Ruelle & Kesselring 1997)

Density (g/cm³):
- 321.0 (calculated-Le Bas method at normal boiling point)
- 244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.206 (mp at 95°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 2.73 × 10^{-3}; 4.33 × 10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)
- 2.73 × 10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C):
- 8.71 × 10^{-5} (supercooled liquid Pₐ, GC-RT correlation, Kurz & Ballschmiter 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 12.02 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
- 6.82 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
- 9.13 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_{B}:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:
- Biota: biological t_{1/2} > 170 d (range 100 to > 300 d) in rainbow trout (average value for hexachloro-DPE congeners, Niimi 1986)
10.1.4.19 2,2',3,4,4',5-Hexachlorodiphenyl ether (PCDE-137)

Common Name: 2,2',3,4,4',5-Hexachlorodiphenyl ether
Synonym: PCDE-137
Chemical Name: 2,2',3,4,4',5-hexachlorodiphenyl ether
CAS Registry No: 71585-36-9
Molecular Formula: C_{12}H_{4}Cl_{6}O
Molecular Weight: 376.878

Melting Point (°C):
- 78–80 (Navalainen et al. 1994)
- 69 (Ruelle & Kesselring 1997)
- 80 (Passivirta et al. 1999)

Boiling Point (°C):

Density (g/cm³):
- 321.0 (calculated-Le Bas method at normal boiling point)
- 244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):

Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
- 56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
- 0.285 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
- $1.85 \times 10^{-3}$; $2.18 \times 10^{-3}$ (quoted expnl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- $1.61 \times 10^{-3}$ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- $2.0 \times 10^{-4}$ ($P_L$, GC-RT correlation, Kurz & Ballschmiter 1999)
- $2.04 \times 10^{-4}$; $5.80 \times 10^{-5}$ (supercooled liquid $P_L$, GC-RT correlation; converted to solid $P_S$ with fugacity ratio F, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- 54.95 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
- 6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- 6.72, 6.83 (quoted lit., calculated from lit. log $K_{\text{OW}}$ and estimated log $S_L$, Passivirta et al. 1999)
- 7.11 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:
- 8.37 (calculated-$K_{\text{OW}}/K_{AW}$, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log $K_B$: 
Sorption Partition Coefficient, log $K_{OC}$:

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

Half-Lives in the Environment:

- Biota: mean biological $t_{1/2} = 100$ d (range 69–179 d) in rainbow trout, mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.20 2,2′,3,4,4′,5′-Hexachlorodiphenyl ether (PCDE-138)

Common Name: 2,2′,3,4,4′,5′-Hexachlorodiphenyl ether
Synonym: PCDE-138
Chemical Name: 2,2′,3,4,4′,5′-hexachlorodiphenyl ether
CAS Registry No: 71585-38-1
Molecular Formula: C₁₂H₄Cl₆O
Molecular Weight: 376.878
Melting Point (°C): 69–70 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
- 321.0 (calculated-Le Bas method at normal boiling point)
- 244.0 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
- 56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
- 0.359 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
- 1.84 × 10⁻³ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
  log [Sₗ/(mol/L)] = –1.868 – 1014/(T/K) (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 1.70 × 10⁻⁴ (P₁, GC-RT correlation, Kurz & Ballschmiter 1999)
- 1.73 × 10⁻³; 6.23 × 10⁻⁵ (supercooled liquid Pₗ, GC-RT correlation; converted to solid Pₛ with fugacity ratio F, Passivirta et al. 1999)
  log (Pₛ/Pa) = 12.15 – 4866/(T/K) (solid, Passivirta et al. 1999)
  log (Pₗ/Pa) = 9.21 – 3854/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- 34.67 (calculated-P/C, Kurz & Ballschmiter 1999)
  log [H/(Pa m³/mol)] = 11.08 – 2840/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log Kow:
- 7.01 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- 7.01, 6.77 (quoted lit., calculated from lit. log Kow and estimated log Sₗ, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log Koa:
- 8.86 (calculated-Kow/Kaw, Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log Kb:

Sorption Partition Coefficient, log Koc:

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

Half-Lives in the Environment:
- Biota: mean biological t₁/₂ = 100 d (range 69–179 d) in rainbow trout; mean t₁/₂ > 170 d (range 100 to >300 d) for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.21 2,2′,3,4,4′,6′-Hexachlorodiphenyl ether (PCDE-140)

Common Name: 2,2′,3,4,4′,6′-Hexachlorodiphenyl ether
Synonym: PCDE-140
Chemical Name: 2,2′,3,4,4′,6′-hexachlorodiphenyl ether
CAS Registry No: 106220-82-0
Molecular Formula: C_{12}H_{4}Cl_{6}O
Molecular Weight: 376.878
Melting Point (°C):
120–122  (Navalainen et al. 1994)
121  (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
321.0  (calculated-Le Bas method at normal boiling point)
244.0  (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.114 (mp at 121°C)
Water Solubility (g/m³ or mg/L at 25°C):
2.99 × 10⁻³; 6.4 × 10⁻⁴ (quoted exp. corr., calculated-molar volume and mp, Ruelle & Kesselring 1997)
2.99 × 10⁻³ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
2.69 × 10⁻⁴  (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
33.88  (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{OW}:
6.76  (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{OA}:
8.51  (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Biota: mean biological t_{1/2} = 149 d (range 99–302 d) in rainbow trout; mean t_{1/2} > 170 d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.22 2,2′,4,4′,5,5′-Hexachlorodiphenyl ether (PCDE-153)

Common Name: 2,2′,4,4′,5,5′-Hexachlorodiphenyl ether
Synonym: PCDE-153
Chemical Name: 2,2′,4,4′,5,5′-hexachlorodiphenyl ether
CAS Registry No: 71859-30-8
Molecular Formula: C_{12}H_4Cl_6O
Molecular Weight: 376.878
Melting Point (°C):

113–115 (Navalainen et al. 1994)
114 (Ruelle & Kesselring 1997)
115 (Passivirta et al. 1999)

Boiling Point (°C): 
Density (g/cm³):
Molar Volume (cm³/mol):

321.0 (calculated-Le Bas method at normal boiling point)
244.0 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol): 
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.134 (mp at 114°C)
0.126 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):

1.65 × 10⁻⁴; 7.52 × 10⁻⁴ (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.65 × 10⁻⁴ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

log $[S_L/$(mol/L)] = –1.868 – 1047/(T/K)$ (liquid, Passivirta et al. 1999)

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

3.47 × 10⁻⁴ (supercooled liquid $P_L$, GC-RT correlation, Kurz & Ballschmiter 1999)
3.74 × 10⁻⁴; 4.71 × 10⁻⁵ (quoted supercooled liquid $P_L$ from Hinckley et al. 1998; converted to solid $P_S$ with fugacity ratio F, Passivirta et al. 1999)

log ($P_L$/Pa) = 12.19 – 4916/(T/K) (solid, Passivirta et al. 1999)
log ($P_L$/Pa) = 9.24 – 3771/(T/K) (supercooled liquid, Passivirta et al. 1999)

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

79.43 (calculated-P/C, Kurz & Ballschmiter 1999)
log ($H$/Pa·m³/mol) = 11.11 – 2724/(T/K) (Passivirta et al. 1999)

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

6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
6.72, 6.84 (quoted lit., calculated from lit. log $K_{\text{OW}}$ and estimated log $S_L$, Passivirta et al. 1999)

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

8.21 (calculated-$K_{\text{OW}}/K_{\text{AW}}$, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log $K_B$:

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

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

Half-Lives in the Environment:

- Biota: mean biological $t_{1/2} = 167$ d (range 98–553 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.23 2,2′,4,4′,5,6′-Hexachlorodiphenyl ether (PCDE-154)

![Chemical Structure of 2,2′,4,4′,5,6′-Hexachlorodiphenyl ether](image)

Common Name: 2,2′,4,4′,5,6′-Hexachlorodiphenyl ether
Synonym: PCDE-154
Chemical Name: 2,2′,4,4′,5,6′-hexachlorodiphenyl ether
CAS Registry No: 106220-81-9
Molecular Formula: C_{12}H_{4}Cl_{6}O
Molecular Weight: 376.878

Melting Point (°C):
- 94–96 (Navalainen et al. 1994)
- 95 (Ruelle & Kesselring 1997)
- 96 (Passivirta et al. 1999)

Boiling Point (°C):

Density (g/cm³):
- Molar Volume (cm³/mol):
  - 321.0 (calculated-Le Bas method at normal boiling point)
  - 244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- Estimated, Passivirta et al. 1999

Entropy of Fusion, ΔS_{fus} (J/mol K):
- 56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.206 (mp at 95°C)
- 0.198 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
- 3.44 × 10⁻³; 1.16 × 10⁻³ (quoted exp., Le Bas method at normal boiling point)
- 3.44 × 10⁻³ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 6.46 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
- 6.64 × 10⁻⁴; 1.32 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- 70.79 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
- 6.49 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- 6.49, 6.93 (quoted lit., calculated from lit. log K_{OW} and estimated log S_{L}, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
- 8.03 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log $K_B$:

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

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

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 142$ d (range 90–330 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.24 2,3′,4,4′,5,5′-Hexachlorodiphenyl ether (PCDE-167)

Common Name: 2,3′,4,4′,5,5′-Hexachlorodiphenyl ether
Synonym: PCDE-167
Chemical Name: 2,3′,4,4′,5,5′-hexachlorodiphenyl ether
CAS Registry No: 131138-20-0
Molecular Formula: C₁₂H₄Cl₆O
Molecular Weight: 376.878
Melting Point (°C):
   104–105  (Navalainen et al. 1994)
   84      (Ruelle & Kesselring 1997)
   105     (Passivirta et al. 1999)
Boiling Point (°C): 
Density (g/cm³):
Molar Volume (cm³/mol):
   321.0  (calculated-Le Bas method at normal boiling point)
   244.0  (Ruelle & Kesselring 1997; quoted Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
   56.5  (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
   0.161  (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
   7.18 × 10⁻⁴; 1.51 × 10⁻³ (quoted exp., calculated-molar volume, MP and mobile order thermodynamics, Ruelle & Kesselring 1997)
   7.18 × 10⁻⁴ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballenschmiter 1999)

Vapor Pressure (Pa at 25 and reported temperature dependence equations °C):
   2.29 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Kurz & Ballenschmiter 1999)
   2.49 × 10⁻⁴; 4.0 × 10⁻³ (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
   120.23  (calculated-P/C, Kurz & Ballenschmiter 1997)

Octanol/Water Partition Coefficient, log K_{ow}:
   7.11  (RP-HPLC-RI correlation, Kurz & Ballenschmiter 1999)
   7.11, 6.99 (quoted lit., calculated from lit. log K_{ow} and estimated log S_{L}, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, log K_{oa}:
   8.42  (calculated-K_{ow}/K_{aw}, Kurz & Ballenschmiter 1999)

Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log $K_{OC}$:

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

Half-Lives in the Environment:
- Biota: mean biological $t_{1/2} > 170$ d (range 100 to $> 300$ d) in rainbow trout for hexachlorodiphenyl ethers (Niimi 1986).
10.1.4.25 2,2′,3,4,4′,5,5′-Heptachlorodiphenyl ether (PCDE-180)

Common Name: 2,2′,3,4,4′,5,5′-Heptachlorodiphenyl ether
Synonym: PCDE-180
Chemical Name: 2,2′,3,4,4′,5,5′-heptachlorodiphenyl ether
CAS Registry No: 83992-69-2
Molecular Formula: C_{12}H_{3}Cl_{7}O
Molecular Weight: 411.324

Melting Point (°C):
- 88–90 (Navalainen et al. 1994; quoted, Passivirta et al. 1999)
- 89 (Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³):
- 256.9 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
- 341.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 56.5 (estimated, Passivirta et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):
- 0.227 (calculated, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
- 1.30 × 10^{-4}; 4.83 × 10^{-4} (quoted expl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- 1.30 × 10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 6.31 × 10^{-6} (supercooled liquid P_L, GC-RT correlation, Kurz & Ballschmiter 1999)
- 5.14 × 10^{-5}; 1.17 × 10^{-5} (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- 199.53 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
- 7.46 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- 7.46, 7.20 (quoted lit., calculated from lit. log K_{OW} and estimated log S_L, Passivirta et al. 1999)
- 7.39 (GC-RT correlation, Hankenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:
- 8.55 (calculated-K_{OW}/K_{AW}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log $K_b$:

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

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

Half-Lives in the Environment:
- Biota: mean biological $t_{1/2} = 146$ d (range 90–380 d) in rainbow trout; mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
- $t_{1/2} = 6–13$ d for Cl$_7$-DPEs to Cl$_7$-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.26 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether (PCDE-182)

Common Name: 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether
Synonym: PCDE-182
Chemical Name: 2,2',3,4,4',5,6'-heptachlorodiphenyl ether
CAS Registry No: 88467-63-4
Molecular Formula: C₁₂H₃Cl₇O
Molecular Weight: 411.324
Melting Point (°C):
136–138 (Navalainen et al. 1994)
136 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
341.9 (calculated-Le Bas method at normal boiling point)
256.9 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.076 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
log [S L/(mol/L)] = –2.344 – 1215/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.01 × 10⁻⁴; 7.66 × 10⁻⁶ (supercooled liquid P L, GC-RT correlation; converted to solid P S with fugacity ratio F, Passivirta et al. 1999)
log (P L/Pa) = 12.35 – 5188/(T/K) (solid, Passivirta et al. 1999)
log (P L/Pa) = 9.49 – 3976/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
log [H/(Pa m³/mol)] = 11.74 – 2761/(T/K) (Passivirta et al. 1999)
Octanol/Water Partition Coefficient, log K_{ow}:
7.50 (calculated from lit. log K_{ow} and estimated log S L, Passivirta et al. 1999)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
Biota: mean t½ > 300 d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
t½ = 6–13 d for Cl₇-DPEs to Cl₉-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.27 2,2′,3,4,4′,6,6′-Heptachlorodiphenyl ether (PCDE-184)

Common Name: 2,2′,3,4,4′,6,6′-Heptachlorodiphenyl ether
Synonym: PCDE-184
Chemical Name: 2,2′,3,4,4′,6,6′-heptachlorodiphenyl ether
CAS Registry No: 106220-84-2
Molecular Formula: C₁₂H₇Cl₇O
Molecular Weight: 411.324
Melting Point (°C): 142 (calculated, Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
341.9 (calculated-Le Bas method at normal boiling point)
256.9 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
5.6 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.080 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
log [S_I/(mol/L)] = –2.344 – 1227/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.32 × 10⁻⁴; 1.06 × 10⁻³ (supercooled liquid P_L; GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.73 – 5858/(T/K) (solid, Passivirta et al. 1999)
log (P_S/Pa) = 9.78 – 4633/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
log [H/(Pa m³/mol)] = 12.12 – 3406/(T/K) (Passivirta et al. 1999)
Octanol/Water Partition Coefficient, log K_{ ow}:
7.53 (calculated from lit. log K_{ ow} and estimated log S_I, Passivirta et al. 1999)
Octanol/Air Partition Coefficient, log K_{ oA}:
Bioconcentration Factor, log BCF or log K_{ bi}:
Sorption Partition Coefficient, log K_{ oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_½:
Half-Lives in the Environment:
Biota: mean t_½ > 300 d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
t_½ = 6–13 d for Cl₇-DPEs to Cl₉-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.28 2,2′,3,3′,4,4′,5,5′-Octachlorodiphenyl ether (PCDE-194)

Common Name: 2,2′,3,3′,4,4′,5,5′-Octachlorodiphenyl ether
Synonym: PCDE-194
Chemical Name: 2,2′,3,3′,4,4′,5,5′-octachlorodiphenyl ether
CAS Registry No:
Molecular Formula: C₁₂H₂Cl₈O
Molecular Weight: 445.769
Melting Point (°C):
- 125–128 (Navalainen et al. 1994)
- 126 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
- 1.362.8 (calculated-Le Bas method at normal boiling point)
- 2.698 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.102 (mp at 126°C)
Water Solubility (g/m³ or mg/L at 25°C):
- 3.30 × 10⁻⁵; 7.57 × 10⁻⁵ (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
- 3.30 × 10⁻³ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
- 1.74 × 10⁻³ (supercooled liquid P_{L}, GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa-m³/mol at 25°C):
- 234.42 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log K_{ow}:
- 7.78 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log K_{oa}:
- 8.80 (calculated-K_{ow}/K_{aw}, Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
- Biota: t_{1/2} = 6 – 13 d for Cl₇-DPEs to Cl₉-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.29 2,2′,3,3′,4,4′,5,6′-Octachlorodiphenyl ether (PCDE-196)

Common Name: 2,2′,3,3′,4,4′,5,6′-Octachlorodiphenyl ether
Synonym: PCDE-196
Chemical Name: 2,2′,3,3′,4,4′,5,6′-octachlorodiphenyl ether
CAS Registry No: 85918-38-3
Molecular Formula: C_{12}H_{2}Cl_{8}O
Molecular Weight: 445.769
Melting Point (°C):
147–149 (Navalainen et al. 1994)
149 (Passivirta et al. 1999)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
362.8 (calculated-Le Bas method at normal boiling point)
269.8 (Passivirta et al. 1999)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
56.5 (estimated, Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F:
0.0595 (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
log [S_{L}/(mol/L)] = –2.819 – 1247/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.86 × 10⁻⁶; 5.27 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_{L}/Pa) = 12.57 – 5586/(T/K) (solid, Passivirta et al. 1999)
log (P_{L}/Pa) = 9.62 – 4341/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
log [H/(Pa m³/mol)] = 12.44 – 3094/(T/K) (Passivirta et al. 1999)
Octanol/Water Partition Coefficient, log K_{ow}:
7.88 (calculated from lit. log K_{ow} and estimated log S_{L}, Passivirta et al. 1999)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Biota: t_{1/2} = 6 – 13 d for Cl₇-DPEs to Cl₉-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.30 2,2′,3,3′,4,4′,6,6′-Octachlorodiphenyl ether (PCDE-197)

![Chemical Structure](image)

Common Name: 2,2′,3,3′,4,4′,6,6′-Octachlorodiphenyl ether
Synonym: PCDE-197
Chemical Name: 2,2′,3,3′,4,4′,6,6′-octachlorodiphenyl ether
CAS Registry No: 117948-62-6
Molecular Formula: C_{12}H_{2}Cl_{8}O
Molecular Weight: 445.769

Melting Point (°C):
- 124–126 (Navalainen et al. 1994)
- 126 (Passivirta et al. 1999)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):
- 362.8 (calculated-Le Bas method at normal boiling point)
- 269.8 (Passivirta et al. 1999)

Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
- 56.6 (estimated, Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), \( F \):
- 0.100 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
- \( \log \left[ S_{\text{W}}/(\text{mol/L}) \right] = -2.819 - 1179/(T/K) \) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- \( 1.75 \times 10^{-5} \); \( 1.75 \times 10^{-6} \) (supercooled liquid \( P_L \), GC-RT correlation; converted to solid \( P_S \) with fugacity ratio \( F \), Passivirta et al. 1999)
- \( \log (P_L/\text{Pa}) = 12.47 - 5405/(T/K) \) (solid, Passivirta et al. 1999)
- \( \log (P_L/\text{Pa}) = 9.52 - 4228/(T/K) \) (supercooled liquid, Passivirta et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):
- \( \log \left[ H/(\text{Pa m}^3/\text{mol}) \right] = 12.34 - 3049/(T/K) \) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
- 7.73 (calculated from lit. \( \log K_{\text{OW}} \) and estimated \( \log S_{\text{L}} \), Passivirta et al. 1999)

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, \( t_{1/2} \):

Half-Lives in the Environment:
- Biota: \( t_{1/2} = 6 – 13 \) d for Cl_{7}-DPEs to Cl_{9}-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.31 2,2′,3′,4′,5,5′,6-Nonachlorodiphenyl ether (PCDE-206)

Common Name: 2,2′,3′,4′,5,5′,6-Nonachlorodiphenyl ether
Synonym: PCDE-206
Chemical Name: 2,2′,3′,4′,5,5′,6-nonachlorodiphenyl ether
CAS Registry No: 83992-73-8
Molecular Formula: C_{12}H_{Cl9}O
Molecular Weight: 480.214
Melting Point (°C):
176–177 (Navalainen et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
383.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
1.704 \times 10^{-6} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Vapor Pressure (Pa at 25°C):
6.92 \times 10^{-6} (supercooled liquid \( P_L \), GC-RT correlation, Kurz & Ballschmiter 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1949.84 (calculated-P/C, Kurz & Ballschmiter 1999)
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
8.07 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):
8.08 (calculated-\( K_{\text{ow}} / K_{\text{aw}} \), Kurz & Ballschmiter 1999)
Bioconcentration Factor, log BCF or log \( K_b \):
Sorption Partition Coefficient, log \( K_{\text{oc}} \):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{\frac{1}{2}} \):
Half-Lives in the Environment:
Biota: \( t_{\frac{1}{2}} = 6 – 13 \) d for Cl₇-DPEs to Cl₉-DPEs in various tissues of rat (Niimi et al. 1994).
10.1.4.32 Decachlorodiphenyl ether (PCDE-209)

![Chemical Structure of Decachlorodiphenyl Ether]

- **Common Name:** Decachlorodiphenyl ether
- **Synonym:** PCDE-209
- **Chemical Name:** decachlorodiphenyl ether
- **CAS Registry No:** 31710-30-2
- **Molecular Formula:** $C_{12}Cl_{10}O$
- **Molecular Weight:** 514.659
- **Melting Point (°C):**
  - 220–222 (Navalainen et al. 1994)
  - 131 (Ruelle & Kesselring 1997)
- **Boiling Point (°C):**
- **Density (g/cm³):**
- **Molar Volume (cm³/mol):**
  - 404.6 (calculated-Le Bas method at normal boiling point)
  - 295.6 (Ruelle & Kesselring 1997)
- **Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):**
- **Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):**
- **Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$:**
- **Water Solubility (g/m³ or mg/L at 25°C):**
  - $5.64 \times 10^{-8}$; $1.13 \times 10^{-9}$ (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
  - $5.64 \times 10^{-8}$ (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- **Vapor Pressure (Pa at 25°C):**
  - $1.58 \times 10^{-6}$ (supercooled liquid $P_L$, GC-RT correlation, Kurz & Ballschmiter 1999)
- **Henry’s Law Constant (Pa·m³/mol at 25°C):**
  - 14125 (calculated-P/C, Kurz & Ballschmiter 1999)
- **Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:**
  - 8.16 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)
- **Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:**
  - 7.40 (calculated-$K_{\text{OW}}/K_{\text{AW}}$, Kurz & Ballschmiter 1999)
- **Bioconcentration Factor, log $BCF$ or log $K_B$:**
- **Sorption Partition Coefficient, log $K_{\text{OC}}$:**
- **Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:**
- **Half-Lives in the Environment:**
  - Biota: mean biological $t_\text{½} = 46$ d (range 27–164 d) in rainbow trout (Niimi 1986)
10.1.5 Brominated Diphenyl Ethers

10.1.5.1 2-Bromodiphenyl ether (BDE-1)

![Chemical Structure](image)

Common Name: 2-Bromodiphenyl ether  
Synonym: BDE-1, PBDE-1, 1-bromo-2-phenoxybenzene, 2-bromophenyl phenyl ether, o-bromophenyl phenyl ether  
Chemical Name: 2-monobromodiphenyl ether  
CAS Registry No: 7025-06-1  
Molecular Formula: C_{12}H_{9}BrO  
Molecular Weight: 249.103  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
Enthalpy of Vaporization, ΔH_v (kJ/mol):  
63.7  
(estimated by Wong et al. 2001)  
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):  
0.163; 0.163 (supercooled liquid P_L calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
log (P_L/Pa) = –3327/(T/K) + 10.37, (GC-RT correlation, Wong et al. 2001)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log K_{OW}:  
Octanol/Air Partition Coefficient, log K_{OA}:  
7.24; 7.34 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)  
Bioconcentration Factor, log BCF or log K_{BCF}:  
Sorption Partition Coefficient, log K_{OC}:  
Environmental Fate Rate Constants, k, and Half-Lives, t½:  
Half-Lives in the Environment:  
Air: first-order degradation t½ = 50 h (estimated by EPIWIN, Wania & Dugani 2003)  
Surface water: first-order degradation t½ = 900 h (estimated by EPIWIN, Wania & Dugani 2003)  
Ground water:  
Sediment: first-order degradation t½ = 3600 h (estimated by EPIWIN, Wania & Dugani 2003)  
Soil: first-order degradation t½ = 900 h (estimated by EPIWIN, Wania & Dugani 2003)  
Biota:
10.1.5.2 3-Bromodiphenyl ether (BDE-2)

Common Name: 3-Bromodiphenyl ether
Synonym: BDE-2, PBDE-2, 1-bromo-3-phenoxybenzene, 3-bromophenyl phenyl ether, 3-bromophenyl phenyl ether, 3-phenoxybromobenzene, 3-phenoxyphenyl bromide, m-bromodiphenyl ether, m-phenoxybromobenzene, m-phenoxyp phenyl bromide
Chemical Name: 3-monobromodiphenyl ether
CAS Registry No: 6876-00-2
Molecular Formula: C₁₂H₉BrO
Molecular Weight: 249.103
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  218.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
  65.4  (Wong et al. 2001)
Enthalpy of Sublimation, ΔHₛₘ (kJ/mol):
Enthalpy of Fusion, ΔHₖₑₜ (kJ/mol):
Entropy of Fusion, ΔSₖₑₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₖₑₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
  0.128; 0.125 (supercooled liquid Pᵥ: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
  log (Pᵥ/Pₐ) = –3416/(T/K) + 10.56, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₗₒₘₜ:
Octanol/Air Partition Coefficient, log Kₒ₉ₐ:
  7.36; 7.44  (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log Kₒ₉:
Sorption Partition Coefficient, log Kₒₑ:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
10.1.5.3 4-Bromodiphenyl ether (BDE-3)

Common Name: 4-Bromophenyl phenyl ether
Synonym: BDE-3, PBDE-3, \( p \)-bromophenyl phenyl ether, 1-bromo-4-phenoxybenzene, 4-bromophenyl phenyl ether, 4-phenoxybromobenzene, 4-phenoxyphenyl bromide, \( p \)-bromodiphenyl ether, \( p \)-bromophenoxybenzene, \( p \)-phenoxybromobenzene, \( p \)-phenoxyphenyl bromide
Chemical Name: 4-bromodiphenyl ether, bromophenyl ether
CAS Registry No: 101-55-3
Molecular Formula: \( C_{12}H_9BrO \), \( C_6H_5-O-C_6H_4Br \)
Molecular Weight: 249.103
Melting Point (°C):
18.72 (Weast 1977, 1982–83)
18.0 (Dean 1985, 1992)
Boiling Point (°C):
310.1 (Weast 1977, 1982–83)
305 (Dean 1985, 1992)
Density (g/cm³ at 20°C):
1.423 (Dean 1985)
Molar Volume (cm³/mol):
154.8 (20°C, Stephenson & Malanowski 1987)
218.9 (calculated-Le Bas method at normal boiling point)
175.1 (calculated-density)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
47.9 (Tittlemier et al. 2002)
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C, \( F \): 1.0
Water Solubility (g/m³ or mg/L at 25°C):
4.80 (calculated-\( K_{ow} \), Mabey et al. 1982)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.20 (20°C, calculated, Dreisbach 1952; quoted, Callahan et al. 1979; Mabey et al. 1982)
\[ \log (P_t/KPa) = 5.80633 - 1683.84/(–140.25 + T/K), \text{ temp range } 463–673 \text{ K}, \text{ (Antoine eq., Stephenson \& Malanowski 1987)} \]
0.259 (supercooled liquid PL, GC-RT correlation, Tittlemier et al. 2002)
\[ \log (P_t/Pa) = –2503/(T/K) + 7.81, \text{ (Clausius-Clapeyron eq. from GC-RT correlation measurement, Tittlemier et al. 2002)} \]
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):
Octanol/Water Partition Coefficient, log \( K_{ow} \):
4.28 (calculated as per Leo et al. 1971 using data of Branson 1977, Callahan et al. 1979; quoted, Ryan et al. 1988)
4.94 (calculated, Mabey et al. 1982)
5.24 (quoted, Van Leeuwen et al. 1992)
4.85 (estimated, Tittlemier et al. 2002)
Bioconcentration Factor, log BCF:
4.114 (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)

Sorption Partition Coefficient, log $K_{OC}$:
4.623 (sediment-water, calculated-$K_{OC}$, Mabey et al. 1982)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: $<< 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $<< 1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982).
Hydrolysis:
Biodegradation: estimated half-life of 4.0 h in activated sludge, based on biodegradation of 4-chlorophenyl phenyl ether in activated sewage sludge (Branson 1978; quoted, Callahan et al. 1979).
Biotransformation: estimated rate constant of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for the bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:
10.1.5.4 2,4-Dibromodiphenyl ether (BDE-7)

Common Name: 2,4-Dibromodiphenyl ether
Synonym: BDE-7, PBDE-7, 2,4-dibromo-1-phenoxybenzene
Chemical Name: 2,4-dibromodiphenyl ether
CAS Registry No: 171977-44-9
Molecular Formula: C₁₂H₈Br₂O
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHᵥ(ab) (kJ/mol):
Enthalpy of Fusion, ΔHᵥus (kJ/mol):
Entropy of Fusion, ΔSᵥus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSᵥus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0168; 0.0153 (supercooled liquid PL: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (Pᵥ/Pᵥa) = –3941/(T/K) + 11.34, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kᵥow:
5.03 (for dibromodiphenyl ethers, RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)
Octanol/Air Partition Coefficient, log Kᵥoa:
8.37; 8.36 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log Kᵥb:
Sorption Partition Coefficient, log Kᵥoc:
Environmental Fate Rate Constants, k, and Half-Lives, τᵥ:
Half-Lives in the Environment:
### 10.1.5.5 2,4′-Dibromodiphenyl ether (BDE-9)

![Chemical Structure](image)

- **Common Name:** 2,4′-Dibromodiphenyl ether
- **Synonym:** BDE-8, PBDE-8, 1-bromo-2-(4-bromophenoxy)-benzene
- **Chemical Name:** 2,4′-dibromodiphenyl ether
- **CAS Registry No:** 147217-71-8
- **Molecular Formula:** C₁₂H₈Br₂O
- **Molecular Weight:** 327.999
- **Melting Point (°C):**
- **Boiling Point (°C):**
- **Density (g/cm³):**
- **Molar Volume (cm³/mol):**
  - 242.2 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Vaporization, ΔHᵥ (kJ/mol):**
  - 76.4 (Wong et al. 2001)
- **Enthalpy of Sublimation, ΔHₘₗ (kJ/mol):**
- **Enthalpy of Fusion, ΔHₙₙ (kJ/mol):**
- **Entropy of Fusion, ΔSₙₙ (J/mol K):**
- **Fugacity Ratio at 25°C (assuming ΔSₙₙ = 56 J/mol K), F:**
- **Water Solubility (g/m³ or mg/L at 25°C):**
  - Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
  - 0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
  - 0.0137; 0.0124 (supercooled liquid PL: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
  - \( \log (P_L/\text{Pa}) = -3991/(T/K) + 11.42 \), (GC-RT correlation, Wong et al. 2001)
- **Henry’s Law Constant (Pa·m³/mol at 25°C):**
- **Octanol/Water Partition Coefficient, log Kₒₖₗ:**
  - 5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  - 5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)
- **Octanol/Air Partition Coefficient, log Kₒₐ:**
  - 8.47; 8.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
- **Bioconcentration Factor, log BCF or log Kᵦ:**
- **Sorption Partition Coefficient, log Kₒₑ:**
- **Environmental Fate Rate Constants, k, and Half-Lives, t₅₀:**
- **Half-Lives in the Environment:**
10.1.5.6 2,6-Dibromodiphenyl ether (BDE-10)

![Chemical Structure](image)

Common Name: 2,6-Dibromodiphenyl ether  
Synonym: BDE-10, PBDE-10, 1,3-dibromo-2-phenoxybenzene  
Chemical Name: 2,6-dibromodiphenyl ether  
CAS Registry No: 51930-04-2  
Molecular Formula: C_{12}H_{8}Br_{2}O  
Molecular Weight: 327.999  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol): 242.2 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, ΔHV (kJ/mol): 73.1 (Wong et al. 2001)  
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
Vapor Pressure (Pa at 25°C and reported temperature dependence equation): 0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989) 0.0277; 0.0256 (supercooled liquid PL: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
\( \log (P_v/P_a) = -3818/(T/K) + 11.25 \) (GC-RT correlation, Wong et al. 2001)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log K_{ow}: 5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989) 5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)  
Octanol/Air Partition Coefficient, log K_{oa}: 8.12; 8.13 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)  
Bioconcentration Factor, log BCF or log K_{b}:  
Sorption Partition Coefficient, log K_{oc}:  
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:  
Half-Lives in the Environment:
10.1.5.7 3,4-Dibromodiphenyl ether (BDE-12)

Common Name: 3,4-Dibromodiphenyl ether
Synonym: BDE-12, PBDE-12, 1,2-dibromo-4-phenoxybenzene
Chemical Name: 3,4-dibromodiphenyl ether
CAS Registry No: 189084-59-1
Molecular Formula: C₁₂H₈Br₂O
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   242.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
   77.4 (Wong et al. 2001)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
   0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
   0.0119; 0.107 (supercooled liquid P_l: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_l/Pa) = –4020/(T/K) + 11.56, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log KOW:
   5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
   5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)
Octanol/Air Partition Coefficient, log KOA:
   8.55; 8.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log KB:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
10.1.5.8  3,4′-Dibromodiphenyl ether (BDE-13)

Common Name: 3,4′-Dibromodiphenyl ether
Synonym: BDE-13, PBDE-13, 1-bromo-3-(4-bromophenoxy)-benzene
Chemical Name: 3,4′-dibromodiphenyl ether
CAS Registry No: 83694-71-7
Molecular Formula: C₁₂H₈Br₂O
Molecular Weight: 327.999
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  242.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
  77.0  (Wong et al. 2001)
Enthalpy of Sublimation, ∆Hₛₜₜ (kJ/mol):
Enthalpy of Fusion, ∆Hₕₜₜ (kJ/mol):
Entropy of Fusion, ∆Sₕₜₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕₜₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
  0.0188–0.0127  (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
  0.0113; 0.0101  (supercooled liquid Pᵥ, calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
  log (Pᵥ/Pa) = –4044/(T/K) + 11.62,  (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒₜₕ:
  5.03  (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  5.03  (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)
Octanol/Air Partition Coefficient, log Kₒₐₕ:
  8.57; 8.54  (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log Kᵦᵢ:
Sorption Partition Coefficient, log Kₒₑₜ:
Environmental Fate Rate Constants, k, and Half-Lives, tᵦᵢ:
Half-Lives in the Environment:
10.1.5.9 4,4′-Dibromodiphenyl ether (BDE-15)

Common Name: 4,4′-Dibromodiphenyl ether
Synonym: BDE-15, PBDE-15, 1,1-oxybis[4-bromo]benzene, bis(4-bromophenyl)ether, p, p′-dibromodiphenyl ether
Chemical Name: 4,4′-dibromodiphenyl ether
CAS Registry No: 2050-47-7
Molecular Formula: C_{12}H_8Br_2O
Molecular Weight: 327.999

Melting Point (°C):
- 57–58 (Tittlemier et al. 2002)
- 57.7 (Wania & Dugani 2003)

Boiling Point (°C): 242.2 (calculated-Le Bas method at normal boiling point)

Density (g/cm³):

Molar Volume (cm³/mol):

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 78.0 (Wong et al. 2001)
- 67.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):

Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):

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

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:
- 0.477 (mp at 57.5°C, Wania & Dugani 2003)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.130 (generator column-GC/ECD, Tittlemier et al. 2002)
- 0.273, 0.79 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
- 0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
- 9.84 × 10⁻³; 8.80 × 10⁻³ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
- log (P_L/Pa) = –4074/(T/K) + 11.65, (GC-RT correlation, Wong et al. 2001)
- 0.0173 (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)
- log (P_L/Pa) = –3528/(T/K) + 10.08, (Clausius-Clapeyron equation from GC-RT correlation measurements, Tittlemier et al. 2002)
- 0.0143, 0.010 (supercooled, P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 21 (calculated-P_l/C_L, Tittlemier et al. 2002)
- 4.11 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
- 5.03 (value for dibromodiphenyl ether, Pijnenburg et al. 1995)
- 5.55 (estimated, Tittlemier et al. 2002)
- 5.03, 5.48 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, log $K_{oa}$:
- 8.64; 8.60 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.79, 8.63 (selected measured value, final adjusted value, Wania & Dugani 2003)

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

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

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

Volatilization:

Photolysis: photochemical degradation pathway of BDE15 undergoes strict debromination via first-order decay, 
\[ k = 1.98 \times 10^{-2} \text{ min}^{-1} \] in \( 100\% \text{ CH}_3\text{CN} \) and 
\[ k = 3.10 \times 10^{-2} \text{ min}^{-1} \] in \( \text{CH}_3\text{OH} \), corresponding to \( t_{1/2} \approx 30 \text{ min} \) 
(Rayne et al. 2003)

Photooxidation:

Hydrolysis:

Biodegradation: complete debromination under anaerobic microbial degradation in a fixed-film plug-flow bioreactor (Rayne et al. 2003)

Biotransformation:

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

Half-Lives in the Environment:

Air: first order degradation \( t_{1/2} = 120 \text{ h} \) (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation \( t_{1/2} = 1440 \text{ h} \) (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation \( t_{1/2} = 5760 \text{ h} \) (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation \( t_{1/2} = 1440 \text{ h} \) (estimated by EPIWIN, Wania & Dugani 2003)

Biota:
10.1.5.10 2,2′,4-Tribromodiphenyl ether (BDE-17)

Common Name: 2,2′,4-Tribromodiphenyl ether
Synonym: PBDE-17
Chemical Name: 2,2′,4-tribromodiphenyl ether
CAS Registry No: 147217-75-2
Molecular Formula: C₁₂H₇Br₃O
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   0.00038 (calculated for triBDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C at 25°C and reported temperature dependence equation):
   0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
   0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)
   0.00219 (supercooled P₁, GC-RT correlation on a CPSil-8 column, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
   5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
   5.47–5.58 (quoted range of value for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log KOA at 25°C or as indicated and reported temperature dependence equations.
   Additional data at other temperatures designated * are compiled at the end of this section:
   log KOA = –3.54 + 3803/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
Bioconcentration Factor, log BCF or log Kcb:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
### TABLE 10.1.5.10.1
Reported octanol-air partition coefficients of 2,2',4-tribromodiphenyl ether (PBDE 17) at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>log $K_{OA}$ (Harner &amp; Shoeib 2002)</th>
<th>log $K_{OA}$ (Chen et al. 2002)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-GC/MS</td>
<td>quantitative predictive model</td>
</tr>
<tr>
<td>15</td>
<td>9.777</td>
<td>9.966</td>
</tr>
<tr>
<td>25</td>
<td>9.27</td>
<td>9.385</td>
</tr>
<tr>
<td>35</td>
<td>8.901</td>
<td>8.841</td>
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<tr>
<td>45</td>
<td>8.517</td>
<td>8.332</td>
</tr>
<tr>
<td>25</td>
<td>9.3</td>
<td></td>
</tr>
</tbody>
</table>

QRSETP model 3

$\log K_{OA} = A + B/(T/K)$

- $A = -3.45$
- $B = 3803$

Quantitative relationships between structures, environmental temperatures and properties.

**FIGURE 10.1.5.10.1** Logarithm of $K_{OA}$ versus reciprocal temperature for 2,2',4-tribromodiphenyl ether (PBDE-17).
10.1.5.11 2,4,4′-Tribromodiphenyl ether (BDE-28)

Common Name: 2,4,4′-Tribromodiphenyl ether
Synonym: PBDE-28, 2,4-dibromo-1-(4-bromophenoxy)-benzene, p-bromophenyl 2,4-dibromophenyl ether
Chemical Name: 2,4,4′-tribromodiphenyl ether
CAS Registry No: 41318-75-6
Molecular Formula: C₁₂H₇Br₃O
Molecular Weight: 406.895

Melting Point (°C):
- 64–64.5 (Tittlemier et al. 2002)
- 64.25 (Wania & Dugani 2003)

Boiling Point (°C):

Density (g/cm³):

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

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 94.05 (Tittlemier & Tomy 2001)
- 79.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):

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

Fugacity Ratio at 25°C (assuming $\Delta S_{ fus} = 56$ J/mol K), F:
- 0.409 (at mp 64.25°C, Wania & Dugani 2003)

Water Solubility (g/m³ or mg/L at 25°C):
- 0.00038 (calculated for triBDE, Alcock et al. 1999)
- 0.070 (solid $S_s$, generator column-GC/ECD, Tittlemier et al. 2002)
- 0.173, 0.334 (supercooled liquid $S_L$, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
- 0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
- 0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)
- 1.78 × 10⁻⁴ (supercooled liquid $P_L$: GC-RT correlation, Tittlemier & Tomy 2001)
- $\log(P_L/Pa) = -4912/(T/K) + 12.73$, (GC-RT correlation, Tittlemier & Tomy 2001)
- 0.00160 (supercooled $P_L$: GC-RT correlation on a CPSil-8 column, Wong et al. 2001)
- 2.19 × 10⁻³ (supercooled liquid $P_L$: GC-RT correlation, Tittlemier et al. 2002)
- $\log(P_L/Pa) = -4160/(T/K) + 11.30$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
- 1.96 × 10⁻³, 1.57 × 10⁻³ (supercooled $P_L$, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 5.1 (calculated-$P_L/C_L$, Tittlemier et al. 2002)
- 1.924 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 5.47–5.58 (values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
- 5.98 (estimated from PCDEs and fragment constant, Tittlemier et al. 2002)
- 5.53, 5.80 (selected measured value, final adjusted value, Wania & Dugani 2003)
Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

$9.50^*$ (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -3.54 + 3889/(T/K)$, temp range 15–45°C (generator column-GC, Harner & Shoeib 2002)


9.50, 9.41 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log $K_B$:

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

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

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

$k_2 = 0.019$ d$^{-1}$ with $t_{1/2} = 36.5$ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 128$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 1440$ h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 5760$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 1440$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration $t_{1/2} = 36.5$ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

### TABLE 10.1.5.11.1
Reported octanol-air partition coefficients of 2,4,4′-tribromodiphenyl ether (PBDE 28) at various temperatures

<table>
<thead>
<tr>
<th>Temperature ($t/°C$)</th>
<th>Harner &amp; Shoeib 2002</th>
<th>Chen et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-GC/MS</td>
<td>quantitative predictive model</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$\log K_{OA}$</td>
<td>$\log K_{OA}$</td>
</tr>
<tr>
<td>15</td>
<td>9.994</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>9.46</td>
<td>25</td>
</tr>
<tr>
<td>35</td>
<td>9.077</td>
<td>35</td>
</tr>
<tr>
<td>45</td>
<td>8.709</td>
<td>45</td>
</tr>
<tr>
<td>25</td>
<td>9.5</td>
<td></td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$

$A = -3.54$

$B = 3889$

$\Delta H_{t,\text{OA}}/(\text{kJ mol}^{-1}) = 74.5$

Quantitative relationships between structures, environmental temperatures and properties.
FIGURE 10.1.5.11.1 Logarithm of $K_{OA}$ versus reciprocal temperature for 2,4,4′-tribromodiphenyl ether (PBDE-28).
10.1.5.12 2,4,6-Tribromodiphenyl ether (BDE-30)

![Chemical structure of 2,4,6-Tribromodiphenyl Ether]

Common Name: 2,4,6-Tribromodiphenyl ether
Synonym: PBDE-30, BDE-30, 1,3,5-tribromo-2-phenoxybenzene
Chemical Name: 2,4,6-tribromodiphenyl ether
CAS Registry No: 155999-95-4
Molecular Formula: C₁₂H₇Br₃O
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
85.1 (Wong et al. 2001)
Enthalpy of Sublimation, ΔHₙabh (kJ/mol):
Enthalpy of Fusion, ΔHₙ fus (kJ/mol):
Entropy of Fusion, ΔSₙ fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₙ fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00038 (calculated for triBDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)
4.56 × 10⁻³; 3.96 × 10⁻³ (supercooled liquid Pₖ: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (Pₖ/Pa) = –4232/(T/K) + 11.85, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐw:
5.47–5.58 (tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log Kₐa:
9.02; 8.94 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log Kₐb:
Sorption Partition Coefficient, log Kₐoc:
Environmental Fate Rate Constants, k, and Half-Lives, tₕ:
Half-Lives in the Environment:
10.1.5.13 2,4′,6-Tribromodiphenyl ether (BDE-32)

Common Name: 2,4′,6-Tribromodiphenyl ether
Synonym: PBDE-32, BDE-32, 1,3-dibromo-2-(4-bromophenoxy)-benzene
Chemical Name: 2,4′,6-tribromodiphenyl ether
CAS Registry No: 189083-60-4
Molecular Formula: C_{12}H_{7}Br_{3}O
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
83.3 (Wong et al. 2001)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00038 (calculated for tri-BDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)
2.25 × 10⁻³; 1.90 × 10⁻³ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4352/(T/K) + 11.94, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.59 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log K_{OA}:
9.28; 9.18 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
10.1.5.14 2′,3,4-Tribromodiphenyl ether (BDE-33)

Common Name: 2′,3,4-Tribromodiphenyl ether
Synonym: PBDE-33, BDE-33, 1,2-dibromo-4-(2-bromophenoxy)-benzene
Chemical Name: 2′,3,4-tribromodiphenyl ether
CAS Registry No: 147217-78-5
Molecular Formula: C₁₂H₇Br₃O
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
265.5  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHv (kJ/mol):
81.0  (Wong et al. 2001)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00038  (calculated for tri-BDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150  (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.01150  (estimated for tri-BDE, Alcock et al. 1999)
1.78 × 10⁻³; 1.49 × 10⁻³  (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4443/(T/K) + 12.15, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log KOW:
5.47–5.58  (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58  (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log KOA:
Bioconcentration Factor, log BCF or log KB:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
10.1.5.15  3,3',4-Tribromodiphenyl ether (BDE-35)

Common Name: 3,3',4-Tribromodiphenyl ether
Synonym: PBDE-35, BDE-35, 1,2-dibromo-4-(4-bromophenoxy)-benzene
Chemical Name: 3,3',4-tribromodiphenyl ether
CAS Registry No: 147217-80-9
Molecular Formula: C_{12}H_{7}Br_{3}O
Molecular Weight: 406.895
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
265.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
86.4 (Wong et al. 2001)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00038 (calculated for triBDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.00266–0.00155 (estimated for triBDE, Alcock et al. 1999)
1.39 × 10⁻³; 1.15 × 10⁻³ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4512/(T/K) + 12.28, (GC-RT correlation, Wong et al. 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.47–5.58 (quoted range of values for tribromodiphenyl ethers, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log K_{oa}:
9.61; 9.48 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log K_p:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_½:
Half-Lives in the Environment:
10.1.5.16 3,4,4′-Tribromodiphenyl ether (BDE-37)

![Chemical Structure](image)

Common Name: 3,4,4′-Tribromodiphenyl ether  
Synonym: PBDE-37, BDE-37, 1,2-dibromo-4-(4-bromophenoxy)-benzene  
Chemical Name: 3,4,4′-tribromodiphenyl ether  
CAS Registry No: 147217-81-0  
Molecular Formula: C_{12}H_{7}Br_{3}O  
Molecular Weight: 406.895  
Melting Point (°C):  
Boiling Point (°C):  
Density (g/cm³):  
Molar Volume (cm³/mol):  
Molar Volume (calculated-Le Bas method at normal boiling point): 265.5  
Enthalpy of Vaporization, ΔH_v (kJ/mol): 86.7  
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C): 0.00038  
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):  
Vapor Pressure (Pa at 25°C and reported temperature dependence equation): 0.00266–0.00150  
Vapor Pressure (estimated for tri-BDE, Alcock et al. 1999)  
Vapor Pressure (1.02 × 10⁻³; 8.0 × 10⁻⁴ (supercooled liquid P_l: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001))  
Vapor Pressure (log (P_l/Pa) = −4528/(T/K) + 12.20, (GC-RT correlation, Wong et al. 2001)):  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log K_{OW}:  
Octanol/Water Partition Coefficient, log K_{OW}: 5.47–5.58  
Octanol/Air Partition Coefficient, log K_{OA}:  
Octanol/Air Partition Coefficient, log K_{OA}: 9.68; 9.54  
Bioconcentration Factor, log BCF or log K_{b}:  
Sorption Partition Coefficient, log K_{OC}:  
Environmental Fate Rate Constants, k, and Half-Lives, t_½:  
Half-Lives in the Environment:
10.1.5.17 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47)

![Chemical Structure](image)

Common Name: 2,2',4,4'-Tetrabromodiphenyl ether  
Synonym: PBDE-47, BDE-47, 1,1'-oxybis[2,4-dibromo-benzene], NSC 21724  
Chemical Name: 2,2',4,4'-tetrabromodiphenyl ether  
CAS Registry No: 5436-43-1  
Molecular Formula: C<sub>12</sub>H<sub>6</sub>Br<sub>4</sub>O  
Molecular Weight: 485.791  
Melting Point (°C):  
83.5–84.5 (Tittlemier et al. 2002)  
84.0 (Wania & Dugani 2003)  
Boiling Point (°C):  
Density (g/cm<sup>3</sup>):  
Molar Volume (cm<sup>3</sup>/mol):  
Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):  
103.13 (Tittlemier & Tomy 2001)  
92.0 (Wong et al. 2001)  
94.6 (Tittlemier et al. 2002)  
Enthalpy of Sublimation, ΔH<sub>subl</sub> (kJ/mol):  
Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):  
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:  
0.261 (calculated at mp 84°C, Wania & Dugani 2002)  
Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):  
0.00007 (calculated for tetra-BDE, Alcock et al. 1999)  
0.015 (solid S<sub>S</sub>, generator column-GC/ECD, Tittlemier et al. 2002)  
0.0496, 0.0947 (supercooled liquid S<sub>L</sub>, selected measured value, final adjusted value, Wania & Dugani 2003)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):  
3.35 × 10<sup>–4</sup>–2.60 × 10<sup>–4</sup> (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)  
2.19 × 10<sup>–3</sup> (supercooled liquid P<sub>L</sub>; GC-RT correlation, Tittlemier & Tomy 2001)  
log (P<sub>L</sub>/Pa) = –5386/(T/K) + 13.42, (GC-RT correlation, Tittlemier & Tomy 2001)  
3.19 × 10<sup>–4</sup>; 2.50 × 10<sup>–4</sup> (supercooled P<sub>L</sub>; calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
log (P<sub>L</sub>/Pa) = –4805/(T/K) + 12.62, (GC-RT correlation, Wong et al. 2001)  
1.86 × 10<sup>–4</sup> (supercooled liquid P<sub>L</sub>; GC-RT correlation, Tittlemier et al. 2002)  
log (P<sub>L</sub>/Pa) = –4940/(T/K) + 12.85, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)  
2.66 × 10<sup>–4</sup>, 2.15 × 10<sup>–4</sup> (supercooled P<sub>L</sub>, selected measured value, final adjusted value, Wania & Dugani 2003)  
Henry’s Law Constant (Pa·m<sup>3</sup>/mol at 25°C):  
1.5 (calculated-P/C, Tittlemier et al. 2002)  
1.107 (Wania & Dugani 2003)  
Octanol/Water Partition Coefficient, log K<sub>ow</sub>:  
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)  
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)  
6.02 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)  
6.55 (estimated, Tittlemier et al. 2002)  
6.11, 6.39 (selected measured value, final adjusted value, Wania & Dugani 2003)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.53*  
(generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -6.47 + 5068/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)

10.34; 10.14  
(calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
10.53, 10.44  
(selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log $K_B$:

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

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

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

- $k_1 = 120$ L d$^{-1}$ g$^{-1}$ dry wt, $k_2 = 0.090$ d$^{-1}$ in blue mussels (Gustafsson et al. 1999)
- $k_1 = 0.108$ g org. C g$^{-1}$ lipid h$^{-1}$ in Lake Höytiäinen sediment; 0.251 g org. C g$^{-1}$ lipid h$^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)
- $k_2 = 0.034$ d$^{-1}$ in Lake Höytiäinen sediment; 0.071 d$^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)
- $k_2 = 0.023$ d$^{-1}$ with $t_{1/2} = 30.1$ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

- Air: first order degradation $t_{1/2} = 256$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Surface water: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Ground water:
- Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Biota: depuration half-life of 7.7 d in blue mussels (Gustafsson et al. 1999; biphasic depuration kinetics observed in oligochaete tissues with half-life of 10.5–47.5 h in compartment A for sediment ingesting obliochaetes (Leppänen & Kukkonen 2004)
- depuration $t_{1/2} = 30.1$ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)
### TABLE 10.1.5.17.1
Reported octanol-air partition coefficients of 2,2′,4,4′-tetrabromodiphenyl ether (PBDE 47) at various temperatures

<table>
<thead>
<tr>
<th>Harner &amp; Shoeib 2002</th>
<th>Chen et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>generator column-GC/MS</td>
</tr>
<tr>
<td>t/°C</td>
<td>log K_{OA}</td>
</tr>
<tr>
<td>15</td>
<td>11.129</td>
</tr>
<tr>
<td>25</td>
<td>10.499</td>
</tr>
<tr>
<td>35</td>
<td>10.063</td>
</tr>
<tr>
<td>45</td>
<td>9.428</td>
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<tr>
<td>25</td>
<td>10.53</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
</tbody>
</table>

\[
\log K_{OA} = A + B/(T/K)
\]

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>−6.47</td>
<td>5068</td>
</tr>
</tbody>
</table>

**enthalpy of phase change**

\[
\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 97.0
\]

Quantitative relationships between structures, environmental temperatures and properties.

### FIGURE 10.1.5.17.1
Logarithm of K_{OA} versus reciprocal temperature for 2,2′,4,4′-tetrabromodiphenyl ether (PBDE-47).
**10.1.5.18 2,3',4,4'-Tetrabromodiphenyl ether (BDE-66)**

![Chemical Structure]

**Common Name:** 2,3',4,4'-Tetrabromodiphenyl ether  
**Synonym:** PBDE-66, BDE-66, 1,2-dibromo-4-(2,4-dibromophenoxy)-benzene  
**Chemical Name:** 2,3',4,4'-tetrabromodiphenyl ether  
**CAS Registry No:** 189084-61-5  
**Molecular Formula:** C$_{12}$H$_6$Br$_4$O  
**Molecular Weight:** 485.791

- **Melting Point (°C):**  
- **Boiling Point (°C):**  
- **Density (g/cm$^3$):**  
- **Molar Volume (cm$^3$/mol):** 288.8 (calculated-Le Bas method at normal boiling point)  
- **Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):** 93.5 (Wong et al. 2001)  
- **Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):**  
- **Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:**  

**Water Solubility (g/m$^3$ or mg/L at 25°C):**  
- 0.00007 (calculated for tetraBDE, Alcock et al. 1999)  
- 0.018 (generator column-GC/ECD, Tittlemier et al. 2002)

**Vapor Pressure (Pa at 25°C and reported temperature dependence equation):**  
- $3.35 \times 10^{-4}$–$2.60 \times 10^{-4}$ (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)  
- $2.38 \times 10^{-4}$–$1.90 \times 10^{-4}$ (supercooled liquid $P_L$: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
- $\log (P/P_a) = -4882/(T/K) + 12.75$, (GC-RT correlation, Wong et al. 2001)  
- $1.22 \times 10^{-4}$ (supercooled liquid $P_L$: GC-RT correlation, Tittlemier et al. 2002)  
- $\log (P/P_a) = -5109/(T/K) + 13.23$, (Clausius-Clapeyron eq. form GC-RT correlation, Tittlemier et al. 2002)

**Henry’s Law Constant (Pa·m$^3$/mol at 25°C):**  
- 0.50 (calculated-$P_L/C_L$, Tittlemier et al. 2002)

**Octanol/Water Partition Coefficient, log $K_{ow}$:**  
- 5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)  
- 5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)  
- 6.73 (estimated, Tittlemier et al. 2002)

**Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated and reported temperature dependence equations.**  
**Additional data at other temperatures designated * are compiled at the end of this section:**  
- 10.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)  
- $\log K_{oa} = -7.88 + 5576/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)  
- 10.49; 10.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log \( K_b \);

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

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>Table 10.1.5.18.1</th>
<th>Reported octanol-air partition coefficients of 2,3′,4,4′-tetrabromodiphenyl ether (PBDE-66) at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harner &amp; Shoeib 2002</td>
<td>Generator column-GC/MS</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>log ( K_{OA} )</td>
</tr>
<tr>
<td>15</td>
<td>11.516</td>
</tr>
<tr>
<td>25</td>
<td>10.773</td>
</tr>
<tr>
<td>35</td>
<td>10.224</td>
</tr>
<tr>
<td>45</td>
<td>9.673</td>
</tr>
<tr>
<td>25</td>
<td>10.82 QRSETP model 3</td>
</tr>
<tr>
<td>15</td>
<td>11.281</td>
</tr>
</tbody>
</table>

\( \log K_{OA} = A + B/(T/K) \)

- \( A = -7.88 \)
- \( B = 5576 \)

enthalpy of phase change

\( \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 107.0 \)

Quantitative relationships between structures, environmental temperatures and properties.
10.1.5.19 2,3′,4,6-Tetabromodiphenyl ether (BDE-69)

Common Name: 2,3′,4,6-Tetabromodiphenyl ether
Synonym: PBDE-69, BDE-69, 1,3,5-tribromo-2-(3bromophenoxy)-benzene
Chemical Name: 2,3′,4,6-tetabromodiphenyl ether
CAS Registry No: 327185-09-1
Molecular Formula: C₁₂H₆Br₄O
Molecular Weight: 485.791
Melting Point (°C): 
Boiling Point (°C): 
Density (g/cm³):
Molar Volume (cm³/mol): 288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol): 91.1 (Wong et al. 2001)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfas (kJ/mol):
Entropy of Fusion, ΔSfas (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfas = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):

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

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

Octanol/Water Partition Coefficient, log KOW:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, log KOA:
10.23; 10.04 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log KB:

Sorption Partition Coefficient, log KOC:

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

Half-Lives in the Environment:
10.1.5.20 3,3',4,4'-Tetrabromodiphenyl ether (BDE-77)

![Chemical Structure of 3,3',4,4'-Tetrabromodiphenyl Ether]

Common Name: 3,3',4,4'-Tetrabromodiphenyl ether
Synonym: PBDE-77, BDE-77, 1,1'-xylib[x2,3-dibromophenoxy]-benzene
Chemical Name: 3,3',4,4'-tetrabromodiphenyl ether
CAS Registry No: 93703-48-1
Molecular Formula: C_{12}H_{6}Br_{4}O
Molecular Weight: 485.791
Melting Point (°C): 96.7–98 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
288.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
95.3 (Wong et al. 2001)
98.7 (Tittlemier et al. 2002)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
0.00007 (calculated for tetraBDE, Alcock et al. 1999)
0.006 (generator column-GC/ECD, Tittlemier et al. 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.35 × 10⁻⁴–2.60 × 10⁻⁴ (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
1.56 × 10⁻⁴–1.20 × 10⁻⁴ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_L/Pa) = –4977/(T/K) + 12.89, (GC-RT correlation, Wong et al. 2001)
6.79 × 10⁻⁵ (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/Pa) = –5156/(T/K) + 13.13, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1.2 (calculated-P_L/C_L, Tittlemier et al. 2002)
Octanol/Water Partition Coefficient, log K_{ow}:
5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.96 (estimated, Tittlemier et al. 2002)
Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
10.87* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
11.343, 10.762, 10.218, 9.709 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
11.218, 10.603, 10.097, 9.590 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
10.70; 10.46 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log $K_B$:

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

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

Half-Lives in the Environment:

**TABLE 10.1.5.20.1**

Reported octanol-air partition coefficients of 3,3',4,4'-tetrabromodiphenyl ether (PBDE 77) at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>log $K_{OA}$</th>
<th>QRSETP model 3</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>11.486</td>
<td></td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>10.829</td>
<td></td>
<td>25</td>
</tr>
<tr>
<td>35</td>
<td>10.371</td>
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<td>35</td>
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<tr>
<td>45</td>
<td>9.844</td>
<td></td>
<td>45</td>
</tr>
<tr>
<td>25</td>
<td>10.87</td>
<td>QRSETP model 5</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>35</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>45</td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$

A = -5.69

B = 4936

Enthalpy of phase change

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 94.5$

Quantitative relationships between structures, environmental temperatures and properties.

**FIGURE 10.1.5.20.1** Logarithm of $K_{OA}$ versus reciprocal temperature for 3,3',4,4'-tetrabromodiphenyl ether (PBDE-77).
### 10.1.5.21 2,2′,3,3′,4-Pentabromodiphenyl ether (BDE-82)

![Structural formula of 2,2′,3,3′,4-Pentabromodiphenyl ether](image)

**Common Name:** 2,2′,3,3′,4-Pentabromodiphenyl ether  
**Synonym:** PBDE-82, BDE-82, 1,2,3-tribromo-4-(2,3-dibromophenoxy)-benzene  
**Chemical Name:** 2,2′,3,3′,4-pentabromodiphenyl ether  
**CAS Registry No:** 327185-11-5  
**Molecular Formula:** C\(_{12}\)H\(_5\)Br\(_5\)O  
**Molecular Weight:** 564.687  
**Melting Point (°C):**  
**Boiling Point (°C):**  
**Density (g/cm\(^3\)):**  
**Molar Volume (cm\(^3\)/mol):** 312.1 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):** 99.1 (Wong et al. 2001)  
**Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):**  
**Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), \(F\):**  
**Water Solubility (g/m\(^3\) or mg/L at 25°C):** 6.47 × 10\(^{-7}\) (calculated for pentaBDE, Alcock et al. 1999)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equation):**  
7.33 × 10\(^{-5}\)–1.43 × 10\(^{-3}\) (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)  
0.07 (estimated for pentaBDE, Alcock et al. 1999)  
6.47 × 10\(^{-5}\); 4.80 × 10\(^{-5}\) (supercooled liquid \(P_L\): calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
\[\log (P_l/Pa) = -5175/(T/K) + 13.12\] (GC-RT correlation, Wong et al. 2001)  
**Henry’s Law Constant (Pa-m\(^3\)/mol at 25°C):**  
**Octanol/Water Partition Coefficient, log \(K_{ow}\):**  
6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)  
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)  
**Octanol/Air Partition Coefficient, log \(K_{oa}\):** 11.14; 10.86 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)  
**Bioconcentration Factor, log \(BCF\) or log \(K_{bi}\):**  
**Sorption Partition Coefficient, log \(K_{oc}\):**  
**Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):**  
**Half-Lives in the Environment:**
10.1.5.22 2,2',3,4,4'-Pentabromodiphenyl ether (BDE-85)

Common Name: 2,2',3,4,4'-Pentabromodiphenyl ether
Synonym: PBDE-85, BDE-85, 1,2,3-tribromo-4-(2,4-dibromophenoxy)-benzene
Chemical Name: 2,2',3,4,4'-pentabromodiphenyl ether
CAS Registry No: 182346-21-0
Molecular Formula: C_{12}H_{5}Br_{5}O
Molecular Weight: 564.687
Melting Point (°C): 119–121 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol): 312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
110.95 (Tittlemier & Tomy 2001)
110 (Tittlemier et al. 2002)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
6.47 × 10⁻⁷ (calculated for pentaBDE, Alcock et al. 1999)
0.006 (generator column-GC/ECD, Tittlemier et al. 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
7.33 × 10⁻⁵–1.43 × 10⁻⁵ (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for pentaBDE, Alcock et al. 1999)
2.88 × 10⁻⁶ (supercooled liquid P_l: GC-RT correlation, Tittlemier & Tomy 2001)
log (P_l/Pa) = –5795/(T/K) + 13.91, (GC-RT correlation, Tittlemier & Tomy 2001)
2.81 × 10⁻⁵ (supercooled liquid P_l, GC-RT correlation on a CPSil-8 column, Wong et al. 2001)
9.86 × 10⁻⁶ (supercooled liquid P_l: GC-RT correlation, Tittlemier et al. 2002)
log (P_l/Pa) = –5761/(T/K) + 14.43, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.11 (calculated-P_l/C_l, Tittlemier et al. 2002)
Octanol/Water Partition Coefficient, log K_{OW}:
6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
7.03 (estimated, Tittlemier et al. 2002)
Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
11.66* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{OA} = –6.22 + 5331/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
Bioconcentration Factor, log BCF or log $K_B$:

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

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 10.1.5.22.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported octanol-air partition coefficients of $2,2',3,4,4'$-pentabromodiphenyl ether (PBDE 85) at various temperatures</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>log $K_{OA}$</th>
<th>$t/°C$</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>12.312</td>
<td>15</td>
<td>12.131</td>
</tr>
<tr>
<td>25</td>
<td>11.631</td>
<td>25</td>
<td>11.549</td>
</tr>
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<td>35</td>
<td>11.118</td>
<td>35</td>
<td>11.006</td>
</tr>
<tr>
<td>45</td>
<td>10.544</td>
<td>45</td>
<td>10.497</td>
</tr>
<tr>
<td>25</td>
<td>11.66</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$log K_{OA} = A + B/(T/K)$

A –6.22

B 5331

enthalpy of phase change

$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 102.0$

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

**FIGURE 10.1.5.22.1** Logarithm of $K_{OA}$ versus reciprocal temperature for $2,2',3,4,4'$-pentabromodiphenyl ether (PBDE-85).
### 10.1.5.23 2,2′,4,4′,5-Pentabromodiphenyl ether (BDE-99)

![Chemical Structure of 2,2′,4,4′,5-Pentabromodiphenyl Ether](image)

**Common Name:** 2,2′,4,4′,5-Pentabromodiphenyl ether  
**Synonym:** PBDE-99, BDE-99, 1,2,4-tribromo-5-(2,4-dibromophenoxy)-benzene  
**Chemical Name:** 2,2′,4,4′,5-pentabromodiphenyl ether  
**CAS Registry No.:** 60348-60-9  
**Molecular Formula:** $C_{12}H_5Br_5O$  
**Molecular Weight:** 564.687  
**Melting Point (°C):**  
- 90.5–94.5 (Tittlemier et al. 2002)  
- 92.5 (Wania & Dugani 2003)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):** 312.1 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):**  
- 104.80 (Tittlemier & Tomy 2001)  
- 100.2 (Wong et al. 2001)  
- 108 (Tittlemier et al. 2002)  
**Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):**  
**Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):**  
**Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:** 0.215 (at mp 92.5°C, Wania & Dugani 2003)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
- $6.47 \times 10^{-7}$ (calculated for pentaBDE, Alcock et al. 1999)  
- 0.0094 (solid Sₜ, generator column-GC/ECD, Tittlemier et al. 2002)  
- 0.0275, 0.0389 (supercooled Sₗ, selected measured value, final adjusted value, Wania & Dugani 2003)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equation):**  
- $7.33 \times 10^{-5}$–$1.43 \times 10^{-4}$ (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)  
- 0.07 (estimated for pentaBDE, Alcock et al. 1999)  
- $1.26 \times 10^{-5}$ (supercooled liquid Pₗ; GC-RT correlation, Tittlemier & Tomy 2001)  
- $6.82 \times 10^{-5}$; $5.0 \times 10^{-5}$ (supercooled liquid Pₗ; calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)  
- $1.26 \times 10^{-5}$ (supercooled liquid Pₗ; GC-RT correlation, Tittlemier et al. 2002)  
- $4.57 \times 10^{-5}$, $3.63 \times 10^{-5}$ (supercooled Pₗ, selected measured value, final adjusted value, Wania & Dugani 2003)  
**Henry’s Law Constant (Pa·m³/mol at 25°C):**  
- 0.23 (calculated-Pₗ/C₂, Tittlemier et al. 2002)  
- 0.530 (Wania & Dugani 2003)  
**Octanol/Water Partition Coefficient, log $K_{ow}$:**  
- 6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)  
- 6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
6.81 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
7.13 (estimated, Tittlemier et al. 2002)
6.61, 6.76 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
$\log K_{OA} = -4.64 + 4757/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.002, 11.422, 10.881, 10.373 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
11.28; 10.99 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
11.31, 11.26 (selected measured value, final adjusted value, Wania & Dugani 2003)

11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
$\log K_{OA} = A + B/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
$A = -4.64$, $B = 4757$

Additional data at other temperatures designated * are compiled at the end of this section:

11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
$\log K_{OA} = -4.64 + 4757/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.002, 11.422, 10.881, 10.373 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
11.28; 10.99 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
11.31, 11.26 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log $K_B$:

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

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

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
$k_1 = 170 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt}$; $k_2 = 0.123 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)
$k_1 = 0.066 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$; $k_2 = 0.022 \text{ d}^{-1}$ in Lake Höyttäinen sediment; $k_1 = 0.99 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$;
$k_2 = 0.026 \text{ d}^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

Half-Lives in the Environment:
Air: first order degradation $t_\text{1/2} = 467 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first order degradation $t_\text{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
Ground water:
Sediment: first order degradation $t_\text{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
Soil: first order degradation $t_\text{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
Biota: depuration $t_\text{1/2} = 5.6 \text{ d}$ in blue mussels (Gustafsson et al. 1999);
biphasic depuration kinetics observed in oligochaete tissues with $t_\text{1/2} = 10.5–47.5 \text{ h}$ in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

### TABLE 10.1.5.23.1
Reported octanol-air partition coefficients of 2,2′,4,4′,5-pentabromodiphenyl ether (PBDE 99) at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$\log K_{OA}$ (Harner &amp; Shoeib 2002)</th>
<th>$\log K_{OA}$ (Chen et al. 2002)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>11.847</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>11.321</td>
<td>15</td>
</tr>
<tr>
<td>35</td>
<td>10.887</td>
<td>15</td>
</tr>
<tr>
<td>45</td>
<td>10.258</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>11.31</td>
<td>15</td>
</tr>
<tr>
<td>15</td>
<td>12.067</td>
<td>15</td>
</tr>
<tr>
<td>25</td>
<td>11.485</td>
<td>15</td>
</tr>
<tr>
<td>35</td>
<td>10.942</td>
<td>15</td>
</tr>
<tr>
<td>45</td>
<td>10.433</td>
<td>15</td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$\log K_{OA}$ (QRSETP model 3)</th>
<th>$\log K_{OA}$ (QRSETP model 5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>12.067</td>
<td>12.002</td>
</tr>
<tr>
<td>25</td>
<td>11.485</td>
<td>11.422</td>
</tr>
<tr>
<td>35</td>
<td>10.942</td>
<td>10.881</td>
</tr>
<tr>
<td>45</td>
<td>10.433</td>
<td>10.373</td>
</tr>
</tbody>
</table>

$A = -4.64$, $B = 4757$

enthalpy of phase change
$\Delta H_{OA}/(kJ mol^{-1}) = 91.1$

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FIGURE 10.1.5.23.1 Logarithm of $K_{OA}$ versus reciprocal temperature for 2,2′,4,4′,5-pentabromodiphenyl ether (PBDE-99).

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10.1.5.24 2,2′,4,4′,6-Pentabromodiphenyl ether (BDE-100)

Common Name: 2,2′,4,4′,6-Pentabromodiphenyl ether
Synonym: PBDE-100, 1,3,5-tribromo-2-(2,4-dibromophenoxy)-benzene
Chemical Name: 2,2′,4,4′,6-pentabromodiphenyl ether
CAS Registry No: 189084-64-8
Molecular Formula: C₁₂H₅Br₅O
Molecular Weight: 564.687
Melting Point (°C):
- 102 (Tittlemier et al. 2002)
- 110 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
- 312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
- 102 (Tittlemier et al. 2002)
Enthalpy of Sublimation, ∆Hₘₙₙ (kJ/mol):
Enthalpy of Fusion, ∆Hₙₙₙ (kJ/mol):
Entropy of Fusion, ∆Sₙₙₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₙₙₙ = 56 J/mol K), F:
- 0.179 (at mp 100.5°C, Wania & Dugani 2003)
Water Solubility (g/m³ or mg/L at 25°C):
- 0.040 (generator column-GC/ECD, Tittlemier et al. 2002)
- 0.0499, 0.0541 (supercooled Sₙₙ, selected measured value, final adjusted value, Wania & Dugani 2003)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 7.33 × 10⁻⁵–1.43 × 10⁻⁵ (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
- 2.86 × 10⁻³ (supercooled liquid Pₙₙ, GC-RT correlation, Tittlemier et al. 2002)
- log (Pₙₙ/Pₐₐ) = -5.339/(T/K) + 13.37, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
- 3.99 × 10⁻⁵, 3.68 × 10⁻⁵ (supercooled Pₙₙ, selected measured value, final adjusted value, Wania & Dugani 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.069 (calculated-Pₙₙ/Cₙₙ, Tittlemier et al. 2002)
- 0.384 (Wania & Dugani 2003)
Octanol/Water Partition Coefficient, log Kₐₙₐ:
- 6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
- 6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
- 6.86 (estimated, Tittlemier et al. 2002)
- 6.51, 6.53 (selected measured value, final adjusted value, Wania & Dugani 2003)
Octanol/Air Partition Coefficient, log Kₐₐ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
- log Kₐₐ = -7.18 + 5459/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
- 11.758, 11.179, 10.637, 10.130 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

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

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

Half-Lives in the Environment:
- Air: first order degradation $t_{1/2} = 357$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Surface water: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Ground water:
- Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)
- Biota:

### TABLE 10.1.5.24.1

Reported octanol-air partition coefficients of $2,2',4,4',6$-pentabromodiphenyl ether (PBDE 100) at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$\log K_{OA}$</th>
<th>$t/°C$</th>
<th>$\log K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>11.755</td>
<td>15</td>
<td>11.721</td>
</tr>
<tr>
<td>25</td>
<td>11.185</td>
<td>25</td>
<td>11.14</td>
</tr>
<tr>
<td>35</td>
<td>10.509</td>
<td>35</td>
<td>10.596</td>
</tr>
<tr>
<td>45</td>
<td>9.993</td>
<td>45</td>
<td>10.087</td>
</tr>
<tr>
<td>25</td>
<td>11.13</td>
<td>15</td>
<td>11.758</td>
</tr>
</tbody>
</table>

$log K_{OA} = A + B/(T/K)$

| A     | -7.18         | 35    | 10.637        |
| B     | 5459          | 45    | 10.13         |

enthalpy of phase change  
$\Delta H_{oa}/(kJ mol^{-1}) = 105.0$

| note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties. |
FIGURE 10.1.5.24.1 Logarithm of $K_{OA}$ versus reciprocal temperature for 2,2',4,4',6-pentabromodiphenyl ether (PBDE-100).
**10.1.5.25 2,3,4,4′,6-Pentabromodiphenyl ether (BDE-115)**

![Structure of 2,3,4,4′,6-Pentabromodiphenyl ether](image)

**Common Name:** 2,3,4,4′,6-Pentabromodiphenyl ether  
**Synonym:** PBDE-115, BDE-115, 1,2,3,5-tetabromo-4-(4-bromophenoxy)benzene  
**Chemical Name:** 2,3,4,4′,6-pentabromodiphenyl ether  
**CAS Registry No:** 446254-78-0  
**Molecular Formula:** C\textsubscript{12}H\textsubscript{5}Br\textsubscript{5}O  
**Molecular Weight:** 564.687  
**Melting Point (°C):**  
**Boiling Point (°C):**  
**Density (g/cm\textsuperscript{3}):**  
**Molar Volume (cm\textsuperscript{3}/mol):** 312.1 \textsuperscript{(calculated-Le Bas method at normal boiling point)}  
**Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):** 101.8 \textsuperscript{(Wong et al. 2001)}  
**Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):**  
**Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):**  
**Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \(\Delta S_{ fus} = 56\) J/mol K), \(F\):**  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):** 6.47 \times 10^{-7} \textsuperscript{(calculated for penta-BDE, Alcock et al. 1999)}  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equation):**  
7.33 \times 10^{-5}–1.43 \times 10^{-5} \textsuperscript{(for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)}  
0.07 \textsuperscript{(estimated for penta-BDE, Alcock et al. 1999)}  
3.02 \times 10^{-5}; 3.20 \times 10^{-5} \textsuperscript{(supercooled liquid \(P_L\): calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)}  
\log (P_L/\text{Pa}) = -5219/(T/K) + 13.32, \textsuperscript{(GC-RT correlation, Wong et al. 2001)}  
**Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):**  
**Octanol/Water Partition Coefficient, log \(K_{ow}\):** 6.64–6.97 \textsuperscript{(range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)}  
6.64–6.97 \textsuperscript{(quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)}  
**Octanol/Air Partition Coefficient, log \(K_{oa}\) at 25°C:** 11.52; 11.20 \textsuperscript{(calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)}  
**Bioconcentration Factor, log BCF or log \(K_B\):**  
**Sorption Partition Coefficient, log \(K_{OC}\):**  
**Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):**  
**Half-Lives in the Environment:**
10.1.5.26 3,3′,4,4′,5-Pentabromodiphenyl ether (BDE-126)

Common Name: 3,3′,4,4′,5-Pentabromodiphenyl ether
Synonym: PBDE-126, BDE-126, 1,2,3-tribromo-5-(3,4-dibromophenoxy)-benzene
Chemical Name: 3,3′,4,4′,5-pentabromodiphenyl ether
CAS Registry No: 366791-32-4
Molecular Formula: C₁₂H₅Br₅O
Molecular Weight: 564.687
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
312.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
6.47 × 10⁻⁷ (calculated for pentaBDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C):
7.33 × 10⁻⁵–1.43 × 10⁻⁵ (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.07 (estimated for penta-PBDEs, Alcock et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log KOW:
6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log KOA at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
11.97* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log KOA = −8.41 + 6077/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
12.642, 12.001, 11.441, 10.611 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
Bioconcentration Factor, log BCF or log KBC:
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
### TABLE 10.1.5.26.1
Reported octanol-air partition coefficients of 3,3′,4,4′,5-pentabromodiphenyl ether (PBDE 126) at various temperatures

<table>
<thead>
<tr>
<th>Harner &amp; Shoeib 2002</th>
<th>Chen et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>generator column-GC/MS</strong></td>
<td><strong>quantitative predictive model</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>log K\textsubscript{OA}</td>
</tr>
<tr>
<td>15</td>
<td>12.642</td>
</tr>
<tr>
<td>25</td>
<td>12.001</td>
</tr>
<tr>
<td>35</td>
<td>11.441</td>
</tr>
<tr>
<td>45</td>
<td>10.611</td>
</tr>
<tr>
<td>25</td>
<td>11.97</td>
</tr>
<tr>
<td>log K\textsubscript{OA} = A + B/(T/K)</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>-8.41</td>
</tr>
<tr>
<td>B</td>
<td>6077</td>
</tr>
</tbody>
</table>

enthalpy of phase change

\[ \Delta H_{OA} / (kJ \ mol^{-1}) = 116.0 \]

**note:** \textsuperscript{*}QRSETP - quantitative relationships between structures, environmental temperatures and properties.

#### FIGURE 10.1.5.26.1
Logarithm of K\textsubscript{OA} versus reciprocal temperature for 3,3′,4,4′,5-pentabromodiphenyl ether (PBDE-126).

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10.1.5.27 2,3,3',4,4',5'-Hexabromodiphenyl ether (BDE-138)

Common Name: 2,3,3',4,4',5'-Hexabromodiphenyl ether
Synonym: PBDE-138, BDE-138, 1,2,3-tribromo-4-(2,4,5-tribromophenoxy)-benzene
Chemical Name: 2,3,3',4,4',5'-hexabromodiphenyl ether
CAS Registry No: 182677-30-1
Molecular Formula: C_{12}H_{4}Br_{6}O
Molecular Weight: 643.584
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  335.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_{v} (kJ/mol):
  114.06  (Tittlemier & Tomy 2001)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  4.08 × 10^{-6}  (calculated for hexaBDE, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
  9.44 × 10^{-6}–4.22 × 10^{-6}  (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
  0.95–0.99  (estimated for hexa-BDE, Alcock et al. 1999)
  1.51 × 10^{-6}  (supercooled liquid P_{L}: GC-RT correlation, Tittlemier & Tomy 2001)
log (P_{L}/Pa) = -5957/(T/K) + 14.17, (GC-RT correlation, Tittlemier & Tomy 2001)
  1.58 × 10^{-6}  (supercooled liquid P_{L}: GC-RT correlation, Tittlemier et al. 2002)
log (P_{L}/Pa) = -6191/(T/K) + 14.97, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
  6.86–7.93  (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  6.86–7.92  (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
  7.91  (estimated, Tittlemier et al. 2002)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
10.1.5.28. 2,2',4,4',5,5'-Hexabromodiphenyl ether (BDE-153)

Common Name: 2,2',4,4',5,5'-Hexabromodiphenyl ether
Synonym: PBDE-153, BDE-153, 1,1'-oxybis[2,4,5-tribromophenoxy]-benzene
Chemical Name: 2,2',3,3',5,5'-hexabromodiphenyl ether
CAS Registry No: 68631-49-2
Molecular Formula: C_{12}H_4Br_6O
Molecular Weight: 643.583

Melting Point (°C):
- 160–163 (Tittlemier et al. 2002)
- 161.5 (Wania & Dugani 2003)

Boiling Point (°C):

Density (g/cm³):
- 335.4 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm³/mol):

Enthalpy of Vaporization, ΔH_v (kJ/mol):
- 107.6 (Wong et al. 2001)
- 110 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):

Entropy of Fusion, ΔS_{ fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F:
- 0.045 (calculated at mp 161.5°C, Wania & Dugani 2003)

Water Solubility (g/m³ or mg/L at 25°C):
- 4.08 × 10⁻⁶ (calculated for hexaBDE, Alcock et al. 1999)
- 8.70 × 10⁻⁷ (Solid S_v, generator column-GC/ECD, Tittlemier et al. 2002)
- 0.0195, 0.0167 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
- 0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)
- 8.43 × 10⁻⁶; 5.80 × 10⁻⁸ (supercooled liquid P_{L}: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
log (P_{L}/Pa) = −5620/(T/K) + 13.78, (GC-RT correlation, Wong et al. 2001)
- 2.09 × 10⁻⁶ (supercooled liquid P_{L}: GC-RT correlation, Tittlemier et al. 2002)
log (P_{L}/Pa) = −5763/(T/K) + 13.66, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
- 7.58 × 10⁻⁶, 8.87 × 10⁻⁶ (supercooled P_{L}, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.067 (calculated-P_{L}/C_{L}, Tittlemier et al. 2002)
- 0.342 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{ow}:
- 6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
- 7.39 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
- 7.62 (estimated, Tittlemier et al. 2002)
- 7.13, 7.08 (selected measured value, final adjusted value, Wania & Dugani 2003)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

11.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -5.39 + 5131/(T/K)$, temp range 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)


12.15; 11.78 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

11.82, 11.89 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log $K_B$:

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

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

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

$k_1 = 19 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt. in blue mussels (Gustafsson et al. 1999)}$  

$k_2 = 0.086 \text{ d}^{-1} \text{ in blue mussels (Gustafsson et al. 1999)}$  

$k_2 = 0.051 \text{ d}^{-1} \text{ with } t_\frac{1}{2} = 13.6 \text{ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)}$

Half-Lives in the Environment:

Air: first order degradation $t_\frac{1}{2} = 1110 \text{ h (estimated by EPIWIN, Wania & Dugani 2003)}$

Surface water: first order degradation $t_\frac{1}{2} = 3600 \text{ h (estimated by EPIWIN, Wania & Dugani 2003)}$

Ground water:

Sediment: first order degradation $t_\frac{1}{2} = 14400 \text{ h (estimated by EPIWIN, Wania & Dugani 2003)}$

Soil: first order degradation $t_\frac{1}{2} = 3600 \text{ h (estimated by EPIWIN, Wania & Dugani 2003)}$

Biota: depuration $t_\frac{1}{2} = 8.1 \text{ d in blue mussels (Gustafsson et al. 1999)}$;

$t_\frac{1}{2} = 13.6 \pm 9 \text{ d in carp (Stapleton et al. 2004a)}$

Depuration $t_\frac{1}{2} = 13.6 \text{ d (juvenile carp in 100-d experiment Stapleton et al. 2004b)}$

**TABLE 10.1.5.28.1**

Reported octanol-air partition coefficients of 2,2′,4,4′,5,5′-hexabromodiphenyl ether (PBDE 153) at various temperatures

<table>
<thead>
<tr>
<th>Harner &amp; Shoeib 2002</th>
<th>Chen et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-GC/MS</td>
<td>quantitative predictive model</td>
</tr>
<tr>
<td>$t/°\text{C}$</td>
<td>$\log K_{OA}$</td>
</tr>
<tr>
<td>15</td>
<td>12.318</td>
</tr>
<tr>
<td>25</td>
<td>11.86</td>
</tr>
<tr>
<td>35</td>
<td>11.569</td>
</tr>
<tr>
<td>45</td>
<td>10.534</td>
</tr>
<tr>
<td>25</td>
<td>11.82</td>
</tr>
<tr>
<td>15</td>
<td>12.556</td>
</tr>
<tr>
<td>25</td>
<td>11.977</td>
</tr>
<tr>
<td>35</td>
<td>11.435</td>
</tr>
<tr>
<td>45</td>
<td>10.928</td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$  

A $= -5.39$  

B $= 5131$  

enthalpy of phase change  

$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.2$

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.
FIGURE 10.1.5.28.1 Logarithm of $K_{OA}$ versus reciprocal temperature for 2,2',4,4',5,5'-hexabromodiphenyl ether (PBDE-153).
10.1.5.29 2,2′,4,4′,5,6′-Hexabromodiphenyl ether (BDE-154)

Common Name: 2,2′,4,4′,5,6′-Hexabromodiphenyl ether
Synonym: PBDE-154, BDE-154, 1,3,5-tribromo-2-(2,4,5-tribromophenoxy)-benzene
Chemical Name: 2,2′,4,4′,5,6′-hexabromodiphenyl ether
CAS Registry No: 207122-15-4
Molecular Formula: C₁₂H₄Br₆O
Molecular Weight: 643.583
Melting Point (°C): 131–132.5 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  335.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  113 (Tittlemier et al. 2002)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  4.08 × 10⁻⁶ (calculated for hexa-PBDEs, Alcock et al. 1999)
  8.70 × 10⁻⁷ (generator column-GC/ECD, Tittlemier et al. 2002)
Vapor Pressure (Pa at 25°C):
  9.44 × 10⁻⁶–4.22 × 10⁻⁶ (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
  0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)
  3.80 × 10⁻⁶ (supercooled liquid P₇; GC-RT correlation, Tittlemier et al. 2002)
log (P₇/Pa) = −5900/(T/K) + 14.38, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  0.24 (calculated-P₇/C₇, Tittlemier et al. 2002)
Octanol/Water Partition Coefficient, log Kₗ₉ₕ:
  6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
  6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
  7.39 (estimated, Tittlemier et al. 2002)
Octanol/Air Partition Coefficient, log KOA at 25°C or as indicated and reported temperature dependence equations.
  Additional data at other temperatures designated * are compiled at the end of this section
  11.92* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
Bioconcentration Factor, log BCF or log $K_B$;

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

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

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

$k_2 = 2.0 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

Half-Lives in the Environment:

Biota: depuration $t_{1/2} = 35 \pm 18 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

### TABLE 10.1.5.29.1

Reported octanol-air partition coefficients of 2,2′,4,4′,5,6′-hexabromodiphenyl ether (PBDE 154) at various temperatures

<table>
<thead>
<tr>
<th>Harner &amp; Shoeib 2002</th>
<th>Chen et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td>generator column-GC/MS</td>
<td>quantitative predictive model</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$\log K_{OA}$</td>
</tr>
<tr>
<td>15</td>
<td>12.455</td>
</tr>
<tr>
<td>25</td>
<td>11.935</td>
</tr>
<tr>
<td>35</td>
<td>11.531</td>
</tr>
<tr>
<td>45</td>
<td>10.789</td>
</tr>
<tr>
<td>25</td>
<td>11.92</td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$

- $A = -4.62$
- $B = 4931$

enzalp of phase change

$\Delta H_{OA} (\text{kJ mol}^{-1}) = 94.4$

**note:** *QRSETP - quantitative relationships between structures, environmental temperatures and properties.*

---

**FIGURE 10.1.5.29.1** Logarithm of $K_{OA}$ versus reciprocal temperature for 2,2′,4,4′,5,6′-hexabromodiphenyl ether (PBDE-154).
10.1.5.30 2,3',4,4',5-Hexabromodiphenyl ether (BDE-156)

Common Name: 2,3,3',4,4',5-Hexabromodiphenyl ether
Synonym: PBDE-156, BDE-156, 1,2,3,4-tetraabromo-5-(3,4-dibromophenoxy)-benzene
Chemical Name: 2,3,3',4,4',5-hexabromodiphenyl ether
CAS Registry No: 405237-85-6
Molecular Formula: C₁₂H₄Br₆O
Molecular Weight: 643.583
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
335.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₛₘᵢₙ (kJ/mol):
Enthalpy of Fusion, ΔHₕᵢₙ (kJ/mol):
Entropy of Fusion, ΔSₕᵢₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕᵢₙ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
4.08 × 10⁻⁶ (calculated for hexa-PBDEs, Alcock et al. 1999)
Vapor Pressure (Pa at 25°C):
9.44 × 10⁻⁶ – 4.22 × 10⁻⁶ (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)
0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐₙₙ:
6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)
Octanol/Air Partition Coefficient, log Kₐₐ at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
11.97* (generator column-GC/MS, measured range 15–45°C, Harner & Shoebib 2002)
log Kₐₐ = –5.80 + 5298/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoebib 2002)
Bioconcentration Factor, log BCF or log Kₐₐ:
Sorption Partition Coefficient, log Kₐₐ:
Environmental Fate Rate Constants, k, and Half-Lives, tₜₐ:
Half-Lives in the Environment:
# TABLE 10.1.5.30.1
Reported octanol-air partition coefficients of 2,3,3′,4,4′,5′-hexabromodiphenyl ether (PBDE 156) at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K\textsubscript{OA}</th>
<th>Harner &amp; Shoeib 2002 generator column-GC/MS</th>
<th>Chen et al. 2002 quantitative predictive model</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>-</td>
<td>13.211 QRSETP* model 3</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>11.976</td>
<td>12.63 25 QRSETP model 5</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>-</td>
<td>11.577 45 QRSETP model 5</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>10.858</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>11.97</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

\[ \log K_{OA} = A + B/(T/K) \]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K\textsubscript{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>13.15</td>
</tr>
<tr>
<td>25</td>
<td>12.571</td>
</tr>
<tr>
<td>35</td>
<td>12.029</td>
</tr>
<tr>
<td>45</td>
<td>11.522</td>
</tr>
</tbody>
</table>

Enthalpy of phase change:
\[ \Delta H_{OA}/(kJ \text{ mol}^{-1}) = 101.0 \]

Note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

**FIGURE 10.1.5.30.1** Logarithm of K\textsubscript{OA} versus reciprocal temperature for 2,3,3′,4,4′,5′-hexabromodiphenyl ether (PBDE-156).
10.1.5.31 2,2',3,4,5,5',6-Heptabromodiphenyl ether (BDE-183)

Common Name: 2,2',3,4,5,5',6-Heptabromodiphenyl ether
Synonym: PBDE-183, BDE-183, 1,2,3,5-tetrabromo-4-(2,4,5-trobromophenoxy)-benzene
Chemical Name: 2,2',3,4,5,5'-heptabromodiphenyl ether
CAS Registry No: 207122-16-5
Molecular Formula: C_{12}H_{3}Br_{7}O
Molecular Weight: 722.479
Melting Point (°C):
171–173 (Tittlemier et al. 2002)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
358.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
118 (Tittlemier et al. 2002)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.035 (calculated at mp 172°C, Wania & Dugani 2003)
Water Solubility (g/m³ or mg/L at 25°C):
1.50 × 10⁻⁶ (generator column-GC/ECD, Tittlemier et al. 2002)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
4.68 × 10⁻⁷ (supercooled liquid P_L: GC-RT correlation, Tittlemier et al. 2002)
log (P_L/P_a) = –6185/(T/K) + 14.43, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0074 (calculated-P_L/C_L, Tittlemier et al. 2002)
Octanol/Water Partition Coefficient, log K_{ow}:
Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
11.96* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
log K_{oa} = –3.71 + 4672/(T/K), temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
Bioconcentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
Air: first-order degradation t_{1/2} = 1540 h (estimated by EPIWIN, Wania & Dugani 2003)
Surface water: first-order degradation $t_{1/2} = 3600\, \text{h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400\, \text{h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600\, \text{h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

### TABLE 10.1.5.31.1

Reported octanol-air partition coefficients of $2,3,3',4,4',5'$-hexabromodiphenyl ether (PBDE 183) at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$\log K_{OA}$</th>
<th>$t/°C$</th>
<th>$\log K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>-</td>
<td>15</td>
<td>13.263</td>
</tr>
<tr>
<td>25</td>
<td>11.964</td>
<td>25</td>
<td>12.681</td>
</tr>
<tr>
<td>35</td>
<td>11.477</td>
<td>35</td>
<td>12.138</td>
</tr>
<tr>
<td>45</td>
<td>10.978</td>
<td>45</td>
<td>11.628</td>
</tr>
<tr>
<td>25</td>
<td>11.96</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\log K_{OA} = A + B/(T/K)$

A

-3.71

B

4672

enthalpy of phase change

$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 89.5$

**note:** *QRSETP* - quantitative relationships between structures, environmental temperatures and properties.

### FIGURE 10.1.5.31.1

Logarithm of $K_{OA}$ versus reciprocal temperature for $2,2',3,4,4',5'$-heptabromodiphenyl ether (PBDE-183).
10.1.5.32 2',3',4,4',5,6-Heptabromodiphenyl ether (BDE-190)

Common Name: 2',3',4,4',5,6-Heptabromodiphenyl ether
Synonym: PBDE-190, BDE-190, pentabromo-(3,4-dibromophenoxy)-benzene
Chemical Name: 2',3',4,4',5,6-heptabromodiphenyl ether
CAS Registry No: 189084-68-2
Molecular Formula: C\textsubscript{12}H\textsubscript{3}Br\textsubscript{7}O
Molecular Weight: 722.479
Melting Point (°C):
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):

- 358.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
- 121.15 (Tittlemier & Tomy 2001)
- 115.8 (Wong et al. 2001)

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 $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):

Vapor Pressure (Pa at 25°C at 25°C and reported temperature dependence equation):
- $2.34 \times 10^{-7}$ (supercooled liquid $P_L$; GC-RT correlation, Tittlemier & Tomy 2001)
- log ($P_L/P_a$) = $-6327/(T/K) + 14.60$, (GC-RT correlation, Tittlemier & Tomy 2001)
- $9.05 \times 10^{-7}$; $5.70 \times 10^{-7}$ (supercooled liquid $P_L$; calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)
- log ($P_L/P_a$) = $-6048/(T/K) + 14.24$, (GC-RT correlation, Wong et al. 2001)
- $2.82 \times 10^{-7}$ (supercooled liquid $P_L$; GC-RT correlation, Tittlemier et al. 2002)
- log ($P_L/P_a$) = $-6552/(T/K) + 15.44$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):

Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
- 8.36 (estimated, Tittlemier et al. 2002)

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:
10.1.5.33 Decabromodiphenyl ether (BDE-209)

Common Name: Decabromodiphenyl ether
Synonym: PBDE-209, BDE-209, 1,1′-oxybis[2,3,4,5,6-pentabromo]-benzene, bis(pentabromophenyl)-ether, 102(E), 2,2′,3,3′,4,4′,5,5′,6,6′-decabromodiphenyl ether, Decabromobiphenyl oxide, decabromophenyl ether
Chemical Name: decabromodiphenyl ether
CAS Registry No: 1163-19-5
Molecular Formula: C_{12}Br_{10}O
Molecular Weight: 959.167
Melting Point (°C): 302.5 (Wania & Dugani 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
428.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Sublimation, \( \Delta H_{subl} \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
4.17 × 10^{-9} (solid \( S_s \), quoted lit., Wania & Dugani 2003)
Vapor Pressure (Pa at 25°C):
2.95 × 10^{-9} (supercooled liquid \( P_l \), estimated, Wania & Dugani 2003)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{ ow} \):
9.97 (decabromodiphenyl ether, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
9.97 (quoted from Watanabe & Tatsukawa 1990, Pijnenburg et al. 1995)
9.97 (quoted, Wania & Dugani 2003)
Octanol/Air Partition Coefficient, log \( K_{ OA} \):
Bioconcentration Factor, log \( BCF \) or log \( K_b \):
Sorption Partition Coefficient, log \( K_{ OC} \):
Environmental Fate Rate Constant, k, and Half-Lives, \( t_{ 1/2 } \):
Volatilization:
Photolysis: half-lives on different matrices, indoors under artificial UV-light “continuous”: \( t_{ 1/2 } < 0.25 \) h on silica gel, \( t_{ 1/2 } = 12 \) h on sand, \( t_{ 1/2 } = 40–60 \) h on sediment and \( t_{ 1/2 } = 150–200 \) h in soil; for outdoors under sunlight “discontinuous”: \( t_{ 1/2 } = 37 \) h on sand and 80 h on sediment; for outdoor sunlight “continuous”: \( t_{ 1/2 } (calc) = 13 \) h on sand and \( t_{ 1/2 } (calc) = 30 \) on sediment (Söderström et al. 2004)
Photooxidation:
Biodegradation: anaerobic degradation decreased by 30% within 238 d corresponding to a pseudo-first-order \( k = 1 \times 10^{-3} \) d⁻¹ by sewage sludge collected from a mesophilic digester (Gerecke et al. 2005)
Biotransformation:

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

$$k_2 = 1.4 \times 10^{-2} \text{ d}^{-1} \text{ with } t_{1/2} = 50 \text{ d} \text{ in juvenile carp (Stapleton et al. 2004)}$$

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 7620 \text{ h} \text{ (estimated by EPIWIN, Wania & Dugani 2003)}$

Surface water: first order degradation $t_{1/2} = 3600 \text{ h} \text{ (estimated by EPIWIN, Wania & Dugani 2003)}$

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h} \text{ (estimated by EPIWIN, Wania & Dugani 2003)}$; photolysis half-lives on different matrices, indoors under artificial UV-light “continuous”: $t_{1/2} = 40–60 \text{ h}$ on sediment; for outdoors under sunlight “discontinuous”: $t_{1/2} = 80 \text{ h}$ on sediment; for outdoor sunlight “continuous”: $t_{1/2} \text{(calc)} = 30 \text{ h}$ on sediment (Söderström et al. 2004)

Soil: first order degradation $t_{1/2} = 3600 \text{ h} \text{ (estimated by EPIWIN, Wania & Dugani 2003)}$; photolysis half-lives on different matrices, indoors under artificial UV-light “continuous”: $t_{1/2} = 12 \text{ h}$ on sand, and 150–200 h in soil; for outdoors under sunlight “discontinuous”: 37 h on sand; for outdoor sunlight “continuous”: $t_{1/2} \text{(calc)} = 13 \text{ h}$ on sand (Söderström et al. 2004)

Biota: depuration $t_{1/2} = 50 \pm 17 \text{ d} \text{ in juvenile carp (Stapleton et al. 2004)}$
### 10.2 SUMMARY TABLES AND QSPR PLOTS

#### TABLE 10.2.1
Summary of physical properties of ethers and halogenated ethers

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Density, ρ g/m³ at 20°C</th>
<th>Molar volume, Vₘ cm³/mol</th>
<th>MW/ρ at 20°C</th>
<th>Le Bas</th>
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<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Dimethyl ether (Methyl ether)</td>
<td>115-10-6</td>
<td>(CH₃)₂O</td>
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<td>Diethyl ether (Ethyl ether)</td>
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<tr>
<td>Di-n-propyl ether</td>
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<td>Epichlorohydrin</td>
<td>106-89-8</td>
<td>C₅H₆ClO</td>
<td>92.524</td>
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<td>118</td>
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<td>154.11</td>
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<td>198.5</td>
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<td>1.1911</td>
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<td>148.2</td>
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<td>0.994</td>
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<td>1.1911</td>
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<td>C₆H₅ClO</td>
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<td>1</td>
<td>1.1911</td>
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<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Density, ρ g/m³ at 20°C</th>
<th>Molar volume, VM cm³/mol</th>
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<tr>
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<td>C₇H₅Cl₃O</td>
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<td>C₇H₅Cl₄O</td>
<td>245.918</td>
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<td>2,3,5,6-Tetrachloroanisole</td>
<td>6936-40-9</td>
<td>C₇H₄Cl₄O</td>
<td>245.918</td>
<td>84</td>
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<td>Veratrole (1,2-Dimethoxybenzene)</td>
<td>91-16-7</td>
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<td>22.5</td>
<td>206</td>
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<td>158.6</td>
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<td>96-09-3</td>
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<td>120.149</td>
<td>–35.6</td>
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* Assuming ∆Sₘₙ = 56 J/mol K.
### TABLE 10.2.2
Summary of selected physical-chemical properties of ethers and halogenated ethers at 25°C

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<thead>
<tr>
<th>Compound</th>
<th>Vapor pressure (P/Pa)</th>
<th>Solubility (S/g/m³)</th>
<th>Henry's law constant ((H/(\text{Pa} \cdot \text{m}^3/\text{mol}))) calculated P/C</th>
<th>log (K_{\text{OW}})</th>
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<tbody>
<tr>
<td><strong>Aliphatic ethers:</strong></td>
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<td></td>
<td></td>
</tr>
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<td>Dimethyl ether (Methyl ether)</td>
<td>600000</td>
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<td>7662</td>
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<td>3306</td>
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<th>C°/(mol/m³)</th>
<th>Cτ/(mol/m³)</th>
<th>log K_ow</th>
<th>Henry's law constant H/(Pa·m³/mol) calculated P/C</th>
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<td></td>
<td></td>
<td>13.2</td>
<td>0.0624</td>
<td>0.1425</td>
<td>4.02</td>
<td></td>
</tr>
<tr>
<td>2,3,4,5-Tetrachloroanisole</td>
<td></td>
<td></td>
<td>1.35</td>
<td>0.0055</td>
<td>0.0228</td>
<td>4.50</td>
<td></td>
</tr>
<tr>
<td>2,3,5,6-Tetrachloroanisole</td>
<td></td>
<td></td>
<td>1.82</td>
<td>0.0074</td>
<td>0.0280</td>
<td>4.40</td>
<td></td>
</tr>
<tr>
<td>Veratrole (1,2-Dimethoxybenzene)</td>
<td>6690</td>
<td></td>
<td>48.42</td>
<td>48.42</td>
<td></td>
<td>2.18</td>
<td></td>
</tr>
<tr>
<td>4,5-Dichloroveratrole</td>
<td>72</td>
<td></td>
<td>0.2477</td>
<td>0.1287</td>
<td>1.2879</td>
<td>3.11</td>
<td></td>
</tr>
<tr>
<td>3,4,5-Trichloroveratrole</td>
<td>10.3</td>
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<td>0.1077</td>
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<tr>
<td>Tetrachloroveratrole</td>
<td>1.59</td>
<td></td>
<td>0.0058</td>
<td>0.0250</td>
<td></td>
<td>4.86</td>
<td></td>
</tr>
<tr>
<td>Phenetole (Ethoxybenzene)</td>
<td>204</td>
<td>204</td>
<td>569</td>
<td>4.658</td>
<td>4.658</td>
<td>2.68</td>
<td>43.80</td>
</tr>
<tr>
<td>Benzy l ethyl ether</td>
<td>100</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.64</td>
</tr>
<tr>
<td>Styrene oxide</td>
<td>40</td>
<td>40</td>
<td>2800</td>
<td>23.30</td>
<td>23.0</td>
<td>1.61</td>
<td>1.716</td>
</tr>
<tr>
<td>Diphenyl ether</td>
<td>2.93</td>
<td>3.05</td>
<td>18.7</td>
<td>0.1099</td>
<td>0.1146</td>
<td>4.21</td>
<td>26.67</td>
</tr>
</tbody>
</table>

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H/(Pa·m³/mol) = 101325 Pa/C° mol/m³.
### TABLE 10.2.3
Suggested half-life classes of ethers and halogenated ethers in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water* class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aliphatic ethers:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimethyl ether (Methyl ether)</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Diethyl ether (Ethyl ether)</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Methyl t-butyl ether (MTBE)</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Di-n-propyl ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>1,2-Propylene oxide</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Furan</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Tetrahydrofuran</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>1,4-Dioxane</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Halogenated ethers:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chloromethyl methyl ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Bis(chloromethyl)ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Bis(2-chloroethyl)ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Bis(2-chloroisopropyl)ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>2-Chloroethyl vinyl ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Bis(2-chloroethoxy)methane</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Aromatic ethers:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anisole (Methoxybenzene)</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Styrene oxide</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Diphenyl ether</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
</tbody>
</table>

* Certain ethers will have much shorter half-lives because of hydrolysis with singlet oxygen, and biodegradation; this half-life class is conservatively assigned, see Chapter 1 for a discussion.

where,

<table>
<thead>
<tr>
<th>Class</th>
<th>Mean half-life (h)</th>
<th>Range (h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>&lt; 10</td>
</tr>
<tr>
<td>2</td>
<td>17 (~ 1 d)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~ 2 d)</td>
<td>30–100</td>
</tr>
<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
</tr>
<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>7</td>
<td>5500 (~ 8 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>8</td>
<td>17000 (~ 2 years)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>55000 (~ 6 years)</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>
FIGURE 10.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

FIGURE 10.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for ethers.
FIGURE 10.2.3 Octanol-water partition coefficient versus Le Bas molar volume for ethers.

FIGURE 10.2.4 Henry’s law constant versus Le Bas molar volume for ethers.
FIGURE 10.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for ethers.
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Dow Chemical (1979) Personal communication from M. Thomas of Dow Chemical Company to N.W. Gabel of Versar, Inc.


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11 Alcohols

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11.1 LIST OF CHEMICALS AND DATA COMPILATIONS

11.1.1 ALCOHOLS

11.1.1.1 Methanol

Common Name: Methanol
Synonym: methyl alcohol, carbinol, wood alcohol, wood spirit
CAS Registry No: 67-56-1
Molecular Formula: CH₃OH
Molecular Weight: 32.042
Melting Point (°C):
-97.53 (Lide 2003)
Boiling Point (°C):
64.6 (Lide 2003)
Density (g/cm³ at 20°C):
0.7914 (Weast 1982–83)
Molar Volume (cm³/mol):
42.5 (exptl. at normal bp, Lee et al. 1972; quoted, Reid et al. 1977)
40.6 (calculated-density, Rohrschneider 1973)
37.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
Entropy of Fusion, ΔSₘₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Dean 1985; Howard 1990)
miscible (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):
16210* (interpolated-regression of tabulated data, temp range –44.0 to 64.7°C, Stull 1947)
16937* (comparative ebulliometry, measured range 15–83.7°C, Ambrose & Sprake 1970)
log (P/Pa) = 7.18411 – 1569.492/(T/K – 34.613); restricted temp range 15–39°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
log (P/Pa) = 7.20519 – 1581.933/(T/K – 33.439); temp range 15–83.7°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
log (P/mmHg) = [–0.2185 × 8978.8/(T/K)] + 8.639821; temp range –44 to 224°C (Antoine eq., Weast 1972–73)
16958* (static method, measured range 288.15–337.65 K, Gibbard & Creek 1974)
16960 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.24963 – 1806.615/(241.833 + t°C); temp range 1.72–63.38°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 7.20660 – 1582.698/(239.765 + t°C); temp range 14–79.63°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
log (P/kPa) = 7.023029 – 1595.671/(240.905 + t°C), temp range 15–65°C (Antoine eq. derived from exptl data of Gibbard & Creek 1974, Boublik et al. 1984)
16670 (interpolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.89750 – 1474.08/(229.13 + t°C); temp range –14 to 65°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.97328 – 1515.14/(232.85 + t°C); temp range 64–110°C (Antoine eq., Dean 1985, 1992)
16937 (Riddick et al. 1986)
\[
\log (P/\text{kPa}) = 7.20519 - 1581.993/(175.47 + t/\degree\text{C}), \text{temp range not specified (Antoine eq., Riddick et al. 1986)}
\]
\[
\log (P/\text{kPa}) = 7.4182 - 1710.2/(–22.25 + T/\text{K}); \text{temp range 175–273 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.25164 - 1608.39/(–31.07 + T/\text{K}); \text{temp range 274–337 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.09489 - 1521.23/(–39.18 + T/\text{K}); \text{temp range 338–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 5.86277 - 1105.884/(–64.272 + T/\text{K}); \text{temp range 188–228 K (Antoine eq.-IV , Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.44355 - 1712.316/(–22.61 + T/\text{K}); \text{temp range 224–290 K (Antoine eq.-V , Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.26415 - 1615.59/(–30.437 + T/\text{K}); \text{temp range 285–345 K (Antoine eq.-VI, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.14736 - 1544.804/(–37.235 + T/\text{K}); \text{temp range 335–376 K (Antoine eq.-VII, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{kPa}) = 7.27466 - 1641.542/(–25.789 + T/\text{K}); \text{temp range 373–458 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{mmHg}) = 45.6171 – 3.2447 × 10^3/(T/\text{K}) –13.988·\log(T/\text{K}) + 6.6365 × 10^{-3}·(T/\text{K}) – 1.0507 × 10^{–13}·(T/\text{K})^2; \text{temp range 175–513 K (vapor pressure eq., Yaws 1994)}
\]

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

0.446 (partial pressure-isoteniscope, Butler et al. 1935)
0.444 (entrainment method-GC, Burnett 1963)
0.472 (exptl., Hine & Mookerjee 1975)
0.367, 0.319 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
0.45* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
0.451 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
0.704 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
0.451 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
0.620 (gas stripping-GC, Altschuh et al. 1999)
0.506 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

\[
\ln K_{AW} = 8.969 – 5206.8/(T/\text{K}); \text{temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)}
\]

1.239* (40°C, headspace-GC, measured range 40–65°C, Teja et al. 2001)

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

–0.82 (shake flask-CR, Collander 1951)
–0.66 (shake flask-GC, Hansch & Anderson 1967)
–0.77 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
–0.52 (shake flask-RC, Cornford 1982)
–0.70 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
–0.64, –0.63 (quoted, calculated-TSA, Iwase et al. 1985)
–0.71 (shake flask-GC at pH 7.0, Riebesehl & Tomlinson 1986)
–0.74 (recommended, Sangster 1989, 1993)
–0.77 (recommended value, Hansch et al. 1995)

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

2.98* (20.29°C, from GC determined \( \gamma \) in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
2.84 (head-space GC, Abraham et al. 2001)
Bioconcentration Factor, log BCF:

- 4.45 (alga Chlorella fusca, wet wt. basis, Geyer et al. 1984)
- 4.45 (alga Chlorella fusca, calculated-K_{OC}, Geyer et al. 1984)
- < 1.0 (golden ide, after 3 d, Freitag et al. 1985)
- 4.46 (algae, after 1 d, Freitag et al. 1985)
- 2.67 (activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

- -0.23 (calculated-MCI χ, Gerstl & Helling 1987)
- 0.44 (soil, quoted exptl., Meylan et al. 1992)
- -0.36 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- -1.08 (calculated-K_{OW}, Kollig 1993)
- 0.44 (soil, calculated-MCI χ, Sabljic et al. 1995)

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

- Volatilization: t_{1/2} ~ 5.3 h and 2.6 d for a model river 1-m deep and an environmental pond (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_{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} = (5.7 ± 0.6) × 10^8 L mol^{-1} s^{-1} or 9.5 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 292 K (relative rate method, Campbell et al. 1976)
    - k_{OH} = (1.06 ± 0.10) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)
    - k_{OH} = (1.00 ± 0.10) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Ravisankara & Davis 1978)
    - k_{OH} = 5.7 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 300 K (Lyman et al. 1982)
    - k_{OH} = 0.76 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K in air (Meier et al. 1985; quoted, Atkinson 1985)
    - k_{OH}(calc) = 6.5 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 9.0 × 10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)
    - k_{OH} = 0.80 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)
    - k_{OH}(exptl) = 0.90 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = 0.53 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
    - k_{OH} = 8.61 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K (Wallington & Kurylo 1987a)
    - k_{OH} = (9.0 ± 0.9) × 10^{-13} cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = (1.0 ± 0.23) × 10^{-12} cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
    - k_{OH}(calc) = 4.05 × 10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

- Hydrolysis:

- Biodegradation: t_{1/2(aerobic)} = 1 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: $t_{1/2} > 9.9$ 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); estimated $t_{1/2} = 17.8$ d in ambient atmosphere (Howard 1990); atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994); calculated lifetimes of 12 d and 1.0 yr for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000).

Surface water: $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Groundwater:

Sediment:

Soil:

Biota:

### TABLE 11.1.1.1.1
Reported vapor pressures of methanol 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>–44.0</td>
<td>133.3</td>
<td>14.899</td>
<td>9815</td>
</tr>
<tr>
<td>–25.3</td>
<td>666.6</td>
<td>19.236</td>
<td>12468</td>
</tr>
<tr>
<td>–16.2</td>
<td>1333</td>
<td>23.323</td>
<td>15519</td>
</tr>
<tr>
<td>–6.0</td>
<td>2666</td>
<td>27.083</td>
<td>18858</td>
</tr>
<tr>
<td>5.0</td>
<td>5333</td>
<td>29.911</td>
<td>21769</td>
</tr>
<tr>
<td>12.1</td>
<td>7999</td>
<td>32.885</td>
<td>25206</td>
</tr>
<tr>
<td>21.2</td>
<td>13332</td>
<td>35.858</td>
<td>29128</td>
</tr>
<tr>
<td>34.8</td>
<td>26664</td>
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<tr>
<td>49.9</td>
<td>53329</td>
<td>45.407</td>
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<tr>
<td>64.7</td>
<td>101325</td>
<td>48.876</td>
<td>52883</td>
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</tbody>
</table>

**summary of literature data**

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P/Pa$</th>
</tr>
</thead>
<tbody>
<tr>
<td>–97.8</td>
<td>–56.428</td>
</tr>
</tbody>
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**Ambrose & Sprake 1970**

<table>
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<td>14.899</td>
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<td>32.885</td>
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**Gibbard & Creek 1974**

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**Antoine eq. for full range**

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</table>

**data also fitted to Cragoe equation, eq. 5 see ref.**
FIGURE 11.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanol.

TABLE 11.1.1.1.2
Reported Henry’s law constants and octanol-air partition coefficients of methanol at various temperatures

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<td>gas stripping-GC</td>
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</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
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<td>enthalpy of transfer:</td>
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<tr>
<td>ΔH/(kJ mol⁻¹) = 41.0</td>
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FIGURE 11.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanol.

FIGURE 11.1.1.3 Logarithm of $K_{OA}$ versus reciprocal temperature for methanol.
11.1.1.2 Ethanol

Common Name: Ethanol  
Synonym: ethyl alcohol, methylcarbinol  
Chemical Name: ethanol, ethyl alcohol  
CAS Registry No: 64-17-5  
Molecular Formula: \( \text{CH}_3\text{CH}_2\text{OH} \)  
Molecular Weight: 46.068  
Melting Point (°C):  
\(-114.14\) (Lide 2003)  
Boiling Point (°C):  
\(78.29\) (Lide 2003)  
Density (g/cm\(^3\)) at 20°C:  
\(0.78933, 0.78505\) (20°C, 25°C, Dreisbach & Martin 1949)  
\(0.7893\) (Weast 1982–83)  
Molar Volume (cm\(^3\)/mol):  
\(58.6\) (calculated-density, Rohrschneider 1973)  
\(59.2\) (calculated-Le Bas method at normal boiling point)  
Acid Dissociation Constant, \(pK_a\):  
\(15.9\) (Riddick et al. 1986)  
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):  
\(5.02\) (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):  
miscible (Dean 1985)  
miscible (Riddick et al. 1986)  
miscible (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):  
\(7314, 7581^*\) (24.4, 24.8°C, measured range 12.80–78.0°C, Kahlbaum 1883)  
\(6906^*\) (22.7°C, static method, measured range 22.7–78°C, Smyth & Engel 1929)  
\(7599\) (gas saturation/air-bubbling method, Washburn & Handorf 1935)  
\(39345^*\) (vapor-liquid equilibrium VLE data, measured range 35–60°C, Scatchard & Raymond 1938)  
\(7538^*\) (interpolated-regression tabulated data, temp range –31.3 to 78.4°C, Stull 1947)  
\(1593, 7869, 29456\) (0, 25, 50°C, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)  
\(7869^*\) (static method, measured range 0–78.553°C, Kretschmer & Wiebe 1949)  
\(\log (P/\text{mmHg}) = 8.11576 – 1595.76/(t/°C + 226.5);\) temp range 0–78.553°C, Kretschmer & Wiebe 1949  
\(\log (P/\text{mmHg}) = 8.24169 – 1652.6/(230 + t/°C)\) (Antoine eq., Dreisbach & Martin 1949)  
\(7870^*\) (comparative ebulliometry, measured range 19.622–43.2°C, Ambrose & Sprake 1970)  
\(\log (P/\text{Pa}) = 7.24739 – 1599.039/(T/K – 46.391);\) temp range 19.6–93.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)  
\(7865\) (vapor-liquid equilibrium VLE data, Polák & Lu 1972)  
\(\log (P/\text{mmHg}) = [−0.2185 \times 9673.6/(T/K)] + 8.827392;\) temp range –31.3–242°C (Antoine eq., Weast 1972–73)  
\(5852, 6665, 9998\) (20, 25, 30°C, Verschueren 1983)  
\(8060\) (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.24222 – 1595.811/(226.448 + t/°C); temp range 19.62–93.48°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 4.11678 – 323.237/(74.916 + t/°C); temp range 12.8–78.2°C (Antoine eq. from reported exptl. data of Kahlbaum 1883, Boublik et al. 1984)

log (P/kPa) = 7.31243 – 1630.868/(229.581 + t/°C); temp range 0–78.55°C (Antoine eq. from reported exptl. data of Kretschmer & Wiebe 1949, Boublik et al. 1984)

log (P/kPa) = 7.16879 – 1552.601/(222.419 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 8.32109 – 1718.10/(237.52 + t/°C); temp range –2 to 100°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.15946 – 1547.464/(–51.941 + T/K); temp range 320–359 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.23347 – 1591.28/(–47.056 + T/K); temp range 292–367 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 8.9391 – 2381.5/(T/K); temp range 210–271 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 8.5224 – 2299/(T/K); temp range 349–374 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.16386 – 1550.006/(–50.941 + T/K); temp range 320–359 K, (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.27664 – 1615.127/(–45.012 + T/K); temp range 292–353 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P/kPa) = 6.95131 – 1423.668/(–63.568 + T/K); temp range 349–374 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

log (P/mmHg) = 23.8442 – 2.8642 × 103/(T/K) –5.0474·log(T/K) + 3.7448 × 10–11·(T/K) + 2.7361 × 10–5·(T/K)2; temp range 159–516 K (vapor pressure eq., Yaws 1994)

17819 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

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

0.520 (partial pressure-isoteniscope, Butler et al. 1935)
0.0118 (partial vapor pressure, concn.-GC, Burnett & Swoboda 1962)
0.4660 (entrainment method-GC, Burnett 1963)
0.637 (exptl.-calculated Cw/C, Hine & Mookerjee 1975)
0.495, 0.472 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.527* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
0.530 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
0.637 (calculated-MCI χ, Nirmalakhandan & Specce 1988)
0.823 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
0.70 (correlated-molecular structure, Russell et al. 1992)
0.542 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
0.593 (solid-phase microextraction SPME-GC, Bartelt 1997)
0.474 (gas stripping-GC, Altschuh et al. 1999)
0.568 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

ln KAW = 10.173 – 5531.6/(T/K); temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)

0.361 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log KAW = 5.576 – 2757/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kow:

–0.32 (shake flask-CR, Collander 1951)
–0.16 (Leo et al. 1969; Hansch & Dunn III 1972)
–0.30 (shake flask-GC, Dillingham et al. 1973)
–0.31 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
–0.22, –0.20 (calculated-f const., Rekker 1977)
–0.18 (shake flask-RC, Cornford 1982)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

-0.20 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
-0.30 (recommended, Sangster 1989, 1993)
-0.25 (thermometric titration, Fujiwara et al. 1991)
-0.29 (calculated-activity coeff. $\gamma$ from UNIFAC, Dallos et al. 1993)
-0.31, −0.22 (recommended value; value at pH 7.2, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

-1.63 (calculated as per Mackay 1982, Schultz et al. 1990)

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

0.09 (calculated- MCI $\chi$, Gerstl & Helling 1987)
0.20 (soil, exp., Meylan et al. 1992)
-0.14 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
0.20 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

Volatile: $t_{1/2} \sim 6$ d from water (estimated, 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 and/or the Arrhenius expression see reference:

$k = 0.01$ M$^{-1}$ s$^{-1}$ for oxidation by RO$_2$ radical at 30°C in aquatic systems with $t_{1/2} = 8 \times 10^4$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
photooxidation $t_{1/2} = 0.24–2.4$ h based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.8 \pm 0.2) \times 10^9$ L mol$^{-1}$ s$^{-1}$ or $3.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)
$k = < 2 \times 10^2$ M$^{-1}$ s$^{-1}$ for oxidation by singlet oxygen in aquatic systems at 25°C with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; Mill 1982)
k$_{OH} = 2 \times 10^9$ L mol$^{-1}$ s$^{-1}$ at 25°C in the atmosphere with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979)
k$_{OH} = (3.74 \pm 0.37) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978)
k$_{OH} = 1.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (Lyman et al. 1982)
k$_{OH} = (2.62 \pm 0.36) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)
k$_{OH} = 1.75 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Meier et al. 1985)

$k(aq.) = (0.37 \pm 0.04)$ M$^{-1}$ s$^{-1}$ for the reaction with O3 in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
k$_{OH} = 2.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)
k$_{OH}^{(calc)} = 3.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(obs.)} = 2.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
k$_{OH}^{(exptl)} = 2.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(calc)} = 3.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
k$_{OH}^{*} = (33.3 \pm 2.3) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurilo 1987a)

$k_{NO3} < 9.0 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)
k$_{OH}^{*} = 3.33 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)
k$_{OH} = 3.33 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(soln) = 3.20 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)
Alcohols 2483

\[ k_{\text{OH}}^* = 3.27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989, 1990)} \]

\[ k_{\text{OH}} = (3.04 \pm 0.25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by pulse radiolysis-UV spectroscopy; } k_{\text{OH}} = (3.46 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ by relative rate method, at 298 \pm 2 K (Nelson et al. 1990)} \]

\[ k_{\text{aq.}} = 0.51 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH 7.2, } k = 0.72 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH 7.3, and } k = 0.77 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH 8.1 for direct reaction with ozone in water at 21°C with } t_{1/2} = 18 \text{ h at pH 7 (Yao & Haag 1991)} \]

\[ k_{\text{OH}}^{\text{calc}} = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1996)} \]

Hydrolysis:

Biodegradation:

\[ t_{1/2}(\text{aq. aerobic}) = 24–168 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Malaney & Gerhold 1969; selected, Howard et al. 1991)} \]

\[ t_{1/2}(\text{aq. anaerobic}) = 96–672 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)} \]

\[ k = 0.0.43–0.055 \text{ h}^{-1} \text{ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).} \]

Biotransformation:

Bioconcentration, Uptake (k\text{u}) and Elimination (k\text{e}) Rate Constants:

Half-Lives in the Environment:

Air: \[ t_{1/2} = 0.24–2.4 \text{ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976); } \]

\[ t_{1/2} \approx 5.9 \text{ d to 4.0 d estimated in the atmosphere (Graedel 1978; quoted, Howard 1990), based on the reaction with a OH radical concentration of } 8 \times 10^6 \text{ molecules/cm}^3 \text{ (Campbell 1976; Lyman et al. 1982; quoted, Howard 1990); } \]

\[ \text{photooxidation } t_{1/2} = 12.2–122 \text{ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991); } \]

\[ \text{calculated lifetimes of } 3.5 \text{ d and } 26 \text{ d for reactions with OH radical, NO}_3 \text{ radical, respectively (Atkinson 2000).} \]

Surface water: \[ \text{photooxidation } t_{1/2} = 334 \text{ d–36.6 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Netu 1967; selected, Howard et al. 1991); } \]

\[ \text{measured rate constants of } 0.51 \text{ M}^{-1} \text{ s}^{-1}, 0.72 \text{ M}^{-1} \text{ s}^{-1}, 0.77 \text{ M}^{-1} \text{ s}^{-1}, \text{ at pH 7.2, 7.3, 8.1, respectively, for direct reaction with ozone in water at } 21^\circ \text{C, with } t_{1/2} = 18 \text{ h at pH 7 (Yao & Haag 1991).} \]

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

Sediment:

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

Biotransformation:

**Biota**

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<tr>
<td><strong>Reported vapor pressures of ethanol at various temperatures and the coefficients for the vapor pressure equations</strong></td>
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</table>

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

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

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

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<thead>
<tr>
<th>Kahlbaum 1883</th>
<th>Scatchard &amp; Raymond 1938</th>
<th>Kretschmer &amp; Wiebe 1949</th>
<th>Ambrose &amp; Sprake 1970</th>
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<td><strong>static method, VLE data</strong></td>
<td><strong>ebulliometry</strong></td>
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<td>t/°C</td>
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<td>t/°C</td>
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<td></td>
</tr>
<tr>
<td>bp/°C</td>
<td>78.4–78.5</td>
<td>mp/°C</td>
<td>–112</td>
</tr>
</tbody>
</table>

**FIGURE 11.1.1.2.1** Logarithm of vapor pressure versus reciprocal temperature for ethanol.
TABLE 11.1.1.2.2
Reported Henry's law constants and octanol-water partition coefficients of ethanol at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m^3/mol)</th>
<th>t/°C</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0688</td>
<td>20</td>
<td>20.29</td>
</tr>
<tr>
<td>25</td>
<td>0.5274</td>
<td>30</td>
<td>3.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>40.4</td>
<td>2.87</td>
</tr>
</tbody>
</table>

enthalpy of transfer: \( \Delta H/(kJ \text{ mol}^{-1}) = 54.392 \)

FIGURE 11.1.1.2.2 Logarithm of Henry's law constant versus reciprocal temperature for ethanol.

FIGURE 11.1.1.2.3 Logarithm of K_{OA} versus reciprocal temperature for ethanol.
11.1.1.3 Propanol (n-Propyl alcohol)

Common Name: Propanol
Synonym: propyl alcohol, 1-propanol, n-propyl alcohol
Chemical Name: propanol, propyl alcohol, n-propyl alcohol
CAS Registry No: 71-23-8
Molecular Formula: C₃H₈O, CH₃CH₂CH₂OH
Molecular Weight: 60.095
Melting Point (°C): 
-124.39 (Lide 2003)
Boiling Point (°C):
97.2 (Lide 2003)
Density (g/cm³ at 20°C):
0.8035 (Weast 1982–83)
0.8037 (Dean 1985)
Molar Volume (cm³/mol):
75.1 (calculated-density, Rohrschneider 1973)
81.4 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK:
19.4 (pKₐ, Riddick et al. 1986)
Enthalpy of Fusion, ΔHₕₛ (kJ/mol):
5.372 (Riddick et al. 1986)
Entropy of Fusion, ΔSₕₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕₛ = 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))
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):
2844 (saturated vapor density-gas saturation, Puck & Wise 1946)
2594* (interpolated-regression of tabulated data, temp range –15 to 97.8°C, Stull 1947)
2720* (ebuliometry-differential thermal analysis, measured range 19.3–97.3°C, Kemme & Kreps 1969)
log (P/mmHg) = 8.18894 – 1690.864/(221.346 + t/°C); temp range 19.3–97.3°C, or pressure range 14.7–758.5 mmHg (Antoine eq., ebuliometry-differential thermal analysis, Kemme & Kreps 1969)
2798* (comparative ebuliometry, measured range 60.2–104.5°C, Ambrose & Sprake 1970)
log (P/Pa) = 6.74390 – 1365.579/(T/K – 82.093); restricted temp range 60.2–81.2°C (Antoine eq., comparative ebuliometry, Ambrose & Sprake 1970)
log (P/Pa) = 6.87613 – 1441.705/(T/K – 74.291); temp range 60.2–104.5°C (Antoine eq., comparative ebuliometry, Ambrose & Sprake 1970)
log (P/Pa) = [−0.2185 × 10⁴21.1/(T/K)] + 8.937293; temp range –15 to 250°C (Antoine eq., Weast 1972–73)
2744 (extrapolated-Anteoine eq., Boublik et al. 1984)
log (P/Pa) = 6.97878 – 1497.734/(204.094 + t/°C); temp range 48.14–94.36°C (Antoine eq. from reported expctl. data of Brown & Smith 1959, Boublik et al. 1984)
log (P/Pa) = 6.87065 – 1438.587/(198.552 + t°C); temp range 60.2–104.6°C (Antoine eq. from reported expctl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
2780 (interpolated-Anteoine eq., Dean 1985)
log (P/mmHg) = 7.84767 – 1499.21/(204.64 + t°C); temp range 2–120°C (Antoine eq., Dean 1985, 1992)
2798 (Riddick et al. 1986)
log (P/kPa) = 6.87613 – 1441.705/(198.859 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
\[
\log (P/kPa) = 6.86874 - 1437.906/(\text{-}74.621 + T/K); \text{ temp range 333–378 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.74195 - 1364.911/(\text{-}82.114 + T/K); \text{ temp range 356–378 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 8.7592 - 2506/(T/K); \text{ temp range 200–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.74403 - 1366.08/(\text{-}81.994 + T/K); \text{ temp range 356–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.87377 - 1440.743/(\text{-}74.344 + T/K); \text{ temp range 333–376 K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.58415 - 1273.365/(\text{-}92.178 + T/K); \text{ temp range 369–407 K (Antoine eq.-VI, Stephenson & Malanowski 1987)}
\]
\[
\log (P/mmHg) = 31.5155 - 3.457 \times 10^3/(T/K) - 7.5235 \cdot \log (T/K) - 4.287 \times 10^{-11} \cdot (T/K)^2; \text{ temp range 124–537 K (vapor pressure eq., Yaws 1994)}
\]
\[
6939 \quad (40^\circ C, \text{ vapor-liquid equilibrium VLE data, DeBord et al. 2002})
\]
\[
9470 \quad (45.43^\circ C, \text{ vapor-liquid equilibrium VLE data, measured range 45.43–58.9^\circ C, Pasanen et al. 2004})
\]
\[
5876 \quad (37.02^\circ C, \text{ ebulliometric method, measured range 310.17–356.7 K, Lubomska & Malanowski 2004})
\]
\[
\log (P/kPa) = 7.21928 - 1629.492/[(T/K) - 57.556]; \text{ temp range 310.17–356.7 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)}
\]

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

- 0.694 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 0.620 (entrainment method-GC, Burnett 1963)
- 0.683 (exptl., Hine & Mookerjee 1975)
- 0.699: 0.710 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
- 0.751* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
- 0.683 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
- 0.925 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 0.683, 0.942 (quoted, correlated-molecular structure, Russell et al. 1992)
- 0.715 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
- 1.034 (solid-phase microextraction SPME-GC, Bartelt 1997)
- 0.372 (wetted-wall column-GC, Altschuh et al. 1999)
- 0.802 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

\[\ln K_{AW} = 11.830 – 5923.2/(T/K); \text{ temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)}\]
\[
0.490 \quad (20^\circ C, \text{ selected from literature experimentally measured data, Staudinger & Roberts 2001})
\]
\[
\log K_{AW} = 6.955 – 3123/(T/K) \quad (\text{van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001})
\]

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

- 0.34 (shake flask-GC, Hansch & Anderson 1967)
- 0.30 (shake flask-GC, Dillingham et al. 1973)
- 0.25 ± 0.01 (shake flask-GC, Leo et al. 1975)
- 0.29 (Hansch & Leo 1979)
- 0.32 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
- 0.25 (recommended, Sangster 1989)
- 0.25 (recommended value, Hansch et al. 1995)

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

- 3.85* (20.29°C, from GC determined \(\gamma^c\) in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
- 3.20 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log \(BCF\):

- –1.069 (calculated as per Mackay 1982, Schultz et al. 1990)
Sorption Partition Coefficient, log $K_{OC}$:

- 0.37 (calculated-MCI $\chi'$, Gerstl & Helling 1987)
- 0.48 (soil, quoted exptl., Meylan et al. 1992)
- 0.12 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 0.48 (soil, calculated-MCI $1/\chi$, Sabljic et al. 1995)

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

**Vamatilization:**

**Photolysis:**

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

- photooxidation $t_{1/2} = 0.24–2.4$ h 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)
- $k_{OH} = (2.3 \pm 0.2) \times 10^9$ L mol$^{-1}$ s$^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)
- $k < 2 \times 10^2$ M$^{-1}$ s$^{-1}$ for the oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)
- $k_{OH} = 2 \times 10^9$ M$^{-1}$ s$^{-1}$ at 25°C with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979; quoted, Mill 1982)
- $k_{OH} = (5.33 \pm 0.53) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)
- $k = (0.37 \pm 0.04)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigne & Bader 1983)
- $k_{OH}(calc) = 5.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 5.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)
- $k_{OH}(exptl) = 5.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(calc) = 5.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
- $k_{OH} = (5.34 \pm 0.29) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)
- $k_{OH} = 5.34 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k$(soln) = $4.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)
- $k_{OH} = 5.34 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ 298 K (recommended, Atkinson 1989, 1990)
- $k_{OH} = (5.64 \pm 0.48) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (5.50 \pm 0.44) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
- $k_{OH}(calc) = 6.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

**Hydrolysis:**

Biodegradation: average rate of biodegradation 71.0 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

**Biotransformation:**

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

**Half-Lives in the Environment:**

Air: $t_{1/2} = 0.24–2.4$ h 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).

Surface water:

Groundwater:

Sediment:

Soil:

Biota
TABLE 11.1.1.3.1
Reported vapor pressures of propanol at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947
Brown & Smith 1959
Kemme & Kreps 1969
Ambrose & Sprake 1970

<table>
<thead>
<tr>
<th>summary of literature data</th>
<th>differential thermal analysis</th>
<th>comparative ebulliometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>–15.0</td>
<td>133.1</td>
<td>48.14</td>
</tr>
<tr>
<td>5.0</td>
<td>666.6</td>
<td>48.16</td>
</tr>
<tr>
<td>14.7</td>
<td>1333</td>
<td>48.18</td>
</tr>
<tr>
<td>25.3</td>
<td>2666</td>
<td>54.52</td>
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<tr>
<td>36.4</td>
<td>5333</td>
<td>61.51</td>
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<tr>
<td>43.5</td>
<td>7999</td>
<td>65.80</td>
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<td>52.8</td>
<td>13332</td>
<td>70.09</td>
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<td>66.8</td>
<td>26664</td>
<td>74.56</td>
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<tr>
<td>82.0</td>
<td>53329</td>
<td>81.11</td>
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<td>97.08</td>
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<td>101393</td>
<td>97.09</td>
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<tr>
<td>86.0</td>
<td>65456</td>
<td>97.3</td>
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<td>91.13</td>
<td>80472</td>
<td>98.513</td>
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<td>94.36</td>
<td>91342</td>
<td>Antoine eq.</td>
</tr>
<tr>
<td>–127</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[\begin{align*}
\Delta H_v/(kJ \text{ mol}^{-1}) \\
\text{at bp} & \quad 56.066
\end{align*}\]

FIGURE 11.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propanol.
TABLE 11.1.1.3.2
Reported Henry’s law constants and octanol-air partition coefficients of propanol at various temperatures

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Snider &amp; Dawson 1985</td>
<td></td>
</tr>
<tr>
<td>gas stripping-GC</td>
<td></td>
</tr>
<tr>
<td>t/°C     H/(Pa m^3/mol)</td>
<td>t/°C log K_{OA}</td>
</tr>
<tr>
<td>0        0.0757</td>
<td>20.29 3.85</td>
</tr>
<tr>
<td>25       0.7512</td>
<td>30.3 3.56</td>
</tr>
</tbody>
</table>

Gruber et al. 1997

<table>
<thead>
<tr>
<th>GC det’d activity coefficient</th>
<th>t/°C log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>enthalpy of transfer:</td>
<td></td>
</tr>
<tr>
<td>ΔH/(kJ mol^{-1}) = 58.576</td>
<td></td>
</tr>
</tbody>
</table>

FIGURE 11.1.1.3.2 Logarithm of Henry’s law constant versus reciprocal temperature for propanol.

FIGURE 11.1.1.3.3 Logarithm of K_{OA} versus reciprocal temperature for propanol.
11.1.1.4 Isopropanol (i-Propyl alcohol)

Common Name: Isopropanol
Synonym: isopropyl alcohol, 2-propanol, i-propyl alcohol, dimethylcarbinol, sec-propylalcohol, perspirit, petrohol, avantine, IPA
Chemical Name: isopropanol, isopropyl alcohol, i-propyl alcohol
CAS Registry No: 67-63-0
Molecular Formula: C₃H₈O, CH₃(CH₃)CHOH
Molecular Weight: 60.095
Melting Point (°C):
-87.9 (Lide 2003)
Boiling Point (°C):
82.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.7812 (25°C, Butler et al. 1935)
0.7855 (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
76.8 (calculated-density, Rohrschneider 1973)
81.4 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
17.1 (Serjeant & Dempsey 1979; Howard 1990)
Enthalpy of Fusion, ΔHₙₕ (kJ/mol):
5.406 (Riddick et al. 1986)
Entropy of Fusion, ΔSₙₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₙₕ = 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; Howard 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):
5866* (static method-isoteniscoppe, measured 0–90°C, Parks & Barton 1928)
5700* (interpolated-regression of tabulated data, temp range –26.1 to 82.5°C, Stull 1947)
5775* (comparative ebulliometry, measured range 52.3–89.2°C, Ambrose & Sprake 1970)
log (P/Pa) = 6.73896 – 1290.345/(T/K – 82.778); restricted temp range 52.3–71.1°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
log (P/Pa) = 6.86618 – 1360.183/(T/K + 75.558); temp range 52.3–89.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
log (P/mmHg) = 8.11778 – 1580.92/(219.6 + t/°C); temp range 0–101°C (Antoine eq., Dean 1985, 1992)
5775 (Riddick et al. 1986)
log (P/kPa) = 6.86618 – 1360.131/(126.36 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P L/kPa) = 6.86087 – 1357.514/(–75.786 + T/K); temp range 325–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P L/kPa) = 6.72348 – 1282.26/(–83.591 + T/K); temp range 347–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P L/kPa) = 9.681 – 2626/(T/K); temp range 195–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P L/kPa) = 6.73782 – 1290.039/(–82.771 + T/K); temp range 347–363 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P L/kPa) = 6.86451 – 1359.473/(–75.592 + T/K); temp range 325–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P L/kPa) = 6.61939 – 1225.439/(–89.774 + T/K); temp range 350–383 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P/mmHg) = 38.2363– 3.5513 × 10^3/(T/K) – 10.031·log(T/K) – 3.474 × 10^–10·(T/K)^2; temp range 185–508 K (vapor pressure eq., Yaws 1994)

13806 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.814 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
0.820 (exptl., Hine & Mookerjee 1975)
1.159, 0.710 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
1.131 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
3.16* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
ln (1/K_{AW}) = –10.6 + 5413/(T/K); temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

Octanol/Water Partition Coefficient, log K_{ow}:
0.14 (Leo et al. 1969; Hansch & Dunn III 1972)
0.05 (shake flask-GC, Dillingham et al. 1973)
0.05 (Hansch & Leo 1985)
0.14 (HPLC-k' correlation, Funasaki et al. 1986)
0.55 (UNIFAC activity coefficient, Banerjee & Howard 1988)
0.05 (recommended, Sangster 1989, 1993)
0.05 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
3.54* (20.29°C, from GC determined γ∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
3.38 (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, $t_\text{1/2}$:

**Volatilization:** the estimated $t_\text{1/2} \sim 3.6$ d for evaporation from water 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

**Photoysis:**
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
  - photooxidation $t_\text{1/2} = 197$ d to 22 yr in water, based on measured rate constant for the reaction with OH radical (Dorfman & Adams 1973; selected, Howard et al. 1991)
  - photooxidation $t_\text{1/2} = 0.24$–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
  - $k < 2 \times 10^5$ M$^{-1}$ s$^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_\text{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)
  - $k_{\text{OH}} = 4.1 \times 10^9$ M$^{-1}$ s$^{-1}$ at 25°C with $t_\text{1/2} = 1.3$ d (Hendry & Kenley 1979; quoted, Mill 1982)
  - $k_{\text{OH}} = (5.48 \pm 0.55) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at $(296 \pm 2)$ K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)
  - $k_{\text{OH}} = 4.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (Lyman et al. 1982)
  - $k = (1.9 \pm 0.2)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2-6 and 20–23°C (Hoigné & Bader 1983)
  - $k_{\text{OH}}(\text{calc}) = 7.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{\text{OH}}(\text{obs.}) = 6.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)
  - $k_{\text{OH}}(\text{exptl}) = 6.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{\text{OH}}(\text{calc}) = 6.6 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
  - $k_{\text{OH}} = (5.81 \pm 0.34) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)
  - $k_{\text{NO}_3} < 2.3 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)
  - $k = 3.20 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)
  - $k_{\text{OH}}(\text{exptl}) = 5.81 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)
  - $k_{\text{OH}} = 5.81 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{\text{OH}}(\text{obs.}) = 3.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
  - $k_{\text{OH}} = 5.21 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
  - $k_{\text{OH}} = (5.69 \pm 1.09) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{\text{OH}} = (5.78 \pm 0.753) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
  - $k_{\text{OH}}(\text{calc}) = 2.90 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

**Hydrolysis:**

**Biodegradation:**
- $k = 52.0$ mg COD g$^{-1}$ h$^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
- $t_\text{1/2} = 24–168$ h, based on unacclimated aerobic aqueous screening test data (Gellman & Heukelekian 1955; Heukelekian & Rand 1955; Price et al. 1974; Takemoto et al. 1981; Wagner 1976; selected, Howard et al. 1991);
- $t_\text{1/2} = 96–672$ h, based on estimated aerobic aqueous biodegradation half-life and unacclimated anaerobic aqueous screening test data (Hou et al. 1983; Sonoda & Seiko 1968; Speece 1983; selected, Howard et al. 1991).

**Biotransformation:**

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

**Half-Lives in the Environment:**
- Air: photooxidation $t_\text{1/2} = 0.24$–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
- photooxidation $t_\text{1/2} = 6.2$–72 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985, 1987; quoted, Howard 1990; selected, Howard et al. 1991).
Surface water: photooxidation $t_{1/2} = 197$ d to 22 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991); $t_{1/2} = 26–168$ h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

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

Sediment:

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

Biota:

Table: Table 11.1.1.4.1

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

<table>
<thead>
<tr>
<th></th>
<th>Parks &amp; Barton 1928</th>
<th>Stull 1947</th>
<th>Ambrose &amp; Sprake 1970</th>
</tr>
</thead>
<tbody>
<tr>
<td>static method/isoteniscope</td>
<td>summary of literature data</td>
<td>comparative ebulliometry</td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
</tr>
<tr>
<td>0</td>
<td>1187</td>
<td>–26.1</td>
<td>133.1</td>
</tr>
<tr>
<td>5</td>
<td>1613</td>
<td>–7.00</td>
<td>666.6</td>
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<td>82.5</td>
<td>101325</td>
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<td>23571</td>
<td>mp/°C</td>
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</tbody>
</table>

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

at 25°C 44.43

at bp 40.166
FIGURE 11.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for isopropanol.

TABLE 11.1.1.4.2
Reported Henry’s law constants and octanol-air partition coefficients of isopropanol at various temperatures

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-GC</td>
<td>equilibrium headspace-GC</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$H/(Pa \cdot m^3/mol)$</td>
</tr>
<tr>
<td>0</td>
<td>0.0811</td>
</tr>
<tr>
<td>25</td>
<td>0.800</td>
</tr>
<tr>
<td>70</td>
<td>15.94</td>
</tr>
<tr>
<td>enthalpy of transfer: $\Delta H/(kJ \cdot mol^{-1}) = 58.576$</td>
<td></td>
</tr>
<tr>
<td>$\ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{(T/K)}$</td>
<td>50.28</td>
</tr>
</tbody>
</table>

Isopropanol ($i$-propyl alcohol): vapor pressure vs. $1/T$

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FIGURE 11.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for isopropanol.

FIGURE 11.1.4.3 Logarithm of $K_{OA}$ versus reciprocal temperature for isopropanol.
11.1.1.5  *n*-Butanol (*n*-Butyl alcohol)

Common Name: *n*-Butanol  
Synonym: 1-butanol, *n*-butyl alcohol, *n*-propylcarbinol  
Chemical Name: *n*-butyl alcohol, 1-butanol  
CAS Registry No: 71-36-3  
Molecular Formula: C₄H₁₀O, CH₃CH₂CH₂CH₂OH  
Molecular Weight: 74.121  
Melting Point (°C):  
-88.6 (Dean 1985; Riddick et al. 1986; Lide 2003)  
Boiling Point (°C):  
117.73 (Lide 2003)  
Density (g/cm³ at 20°C):  
0.80593 (25°C, Butler et al. 1935)  
0.80980 (25°C, Weast 1982–83)  
0.80956, 0.80575 (20°C, 25°C, Riddick et al. 1986)  
Molar Volume (cm³/mol):  
91.7 (calculated-density, Rohrschneider 1973)  
103.6 (calculated-Le Bas method at normal boiling point)  
Acid Dissociation Constant, pKₐ:  
20.89 (Riddick et al. 1986)  
Enthalpy of Fusion, ∆Hᶠus (kJ/mol):  
9.37 (Riddick et al. 1986)  
Entropy of Fusion, ∆Sᶠus (J/mol K):  
56 (estimated, Yalkowsky & Valvani 1980)  
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):  
68120, 79000* (18, 20°C, shake flask-turbidity, Fühner 1924)  
73500* (volumetric method, Hill & Malisoff 1926)  
64000* (20°C, synthetic method, Jones 1929)  
70800* (30°C, vapor liquid equilibrium, measured range 0–105°C, Mueller et al. 1931)  
74500 (gravimetric method, Stockhart & Hull 1931)  
73180 (24.85°C, shake flask-interferometer, Butler et al. 1933)  
73100 (shake flask-cloud point, Butler et al. 1933)  
70000 (26°C, synthetic method, Othmer et al. 1945)  
73320 (shake flask-residue volume, Booth & Everson 1948)  
74100 (shake flask-interferometry, Hansen et al. 1949)  
73000 (shake flask-interferometry, quoted from Butler et al. 1933, Donahue & Bartell 1952)  
75850 (estimated, McGowan 1954)  
78700 (26.7°C, shake flask-turbidity, Skrzc & Murphy 1954)  
74000 (surface tension, Kinoshita et al. 1958)  
70000 (titration, Petriris & Geankopolis 1959)  
75600* (20°C, synthetic method, measured range 0–125°C, von Erichsen 1962)  
77800 (shake flask-GC, Korenman et al. 1974, 1975)  
74000* (shake flask-colorimetric analysis, De Santis et al. 1976)  
70000* (29.8°C, shake flask-refractometry, measured range 29.8–124.6°C, Aoki & Moriyoshi 1978)  
63300 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)  
77000 (Verschueren 1983; Howard 1990)  
74000* (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)  
74500 (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):

800* (24.0°C, static method, measured range 15.1–117.6°C, Kahlbaum 1898)


log (P/mmHg) = 40.2105 – 4100/(T/K) – 10.35·log (T/K); temp range 25–110°C (isoteniscope measurements, Butler et al. 1935)

819 (saturated vapor density-gas saturation, Puck & Wise 1946)

904 (20°C, summary of literature data, temp range –1.2 to 117°C, Stull 1947)

log (P/mmHg) = 8.27488 – 1873.9/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)

10274* (64.56°C, measured range 64.56–117.56°C, Brown & Smith 1959)

log (P/mmHg) = 7.42117 – 1351.555/(179.810 + t°C); temp range 22.6–117.8°C, Kemme & Kreps 1969)

log (P/mmHg) = 7.42117 – 1351.555/(179.810 + t°C); temp range 22.6–117.8°C, or pressure range 5.5–766

mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

910* (comparative ebulliometry, measured range 78.558–125.686°C, Ambrose & Sprake 1970)

log (P/Pa) = 6.41435 – 1262.767/(T/K – 104.445); restricted temp range 78.558–100.74°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.45743 – 1338.769/(T/K – 96.108); temp range 78.558–125.686°C (Antoine eq., comparative ebulliometry, Kemme & Kreps 1969)

log (P/Pa) = 6.41594 – 1264.106/(–104.251 + T/K); temp range 376–397 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/L/kPa) = 6.54723 – 1339.093/(–96.03 + T/K); temp range 351–397 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
Alcohols

905* (298.11 K, static method-Hg manometer, measured range 283.10–323.12 K, Gracia et al. 1992)
998 (calculated-solvatochromic parameters, Banerjee et al. 1990)

\[
\log (P/\text{mmHg}) = 39.6673 - 4.0017 \times 10^3/(T/\text{K}) - 3.2572 \times 10^{-10} (T/\text{K})^2;
\]

temp range 184–563 K (vapor pressure eq., Yaws 1994)

933* (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

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

0.866 (measured partial pressure/mole fraction \(x\) at dilute concn, Butler et al. 1935)
0.731 (entrainment method-GC, Burnett 1963)
0.892 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
0.860; 0.964; 1.057 (exptl.; calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
0.860 (limiting activity coefficient by headspace-GC, Abraham et al. 1987)
4.024* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

\[
\ln (1/K_{\text{AW}}) = -10.2 + 5234/(T/\text{K}); \text{ temp range: } 40–80^\circ\text{C (equilibrium headspace-GC measurements, Kolb et al. 1992)}
\]

0.880 (limiting activity coefficient by headspace-GC, Li & Carr 1993)
0.868 (wetted-wall column-GC, Altschuh et al. 1999)
1.214 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

\[
\ln K_{\text{AW}} = 12.141 – 5982.0/(T/\text{K}); \text{ temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)}
\]

0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

\[
\log K_{\text{AW}} = 6.600 – 3009/(T/\text{K}) (\text{van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001})
\]

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

0.83 (shake flask-CR, Collander 1951)
0.84 (calculated-\(\pi\) constant, Hansch et al. 1968)
0.88 (Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
0.84, 0.86; 0.84 (calculated-fragment const.; calculated-\(\pi\) constant, Rekker 1977)
0.89 (Hansch & Leo 1979)
0.955 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
1.02 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
0.80 (calculated by Rekker’s method, Hanai et al. 1981)
0.79 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
0.76 (calculated from measured activity coeff. \(\gamma\), Wasik et al. 1981)
0.93 (shake flask-RC, Cornford 1982)
0.80 (RP-HPLC-\(k’\) correlation, D’Amboise & Hanai 1982)
0.87 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
0.79 (generator column-GC, Schantz & Martire 1987)
0.80 (calculated from measured activity coeff., \(\gamma\), Schantz & Martire 1987)
0.87 (calculated-\(\gamma\) from UNIFAC, Banerjee & Howard 1988)
0.823, 0.84 (calculated-CLOGP, calculated-M.O. indices, Bodor et al. 1989)
0.84 (recommended, Sangster 1989, 1993)
0.87 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
0.89 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
0.88 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, \(\log BCF\):

−0.439 (calculated as per Mackay 1982, Schultz et al. 1990)
Sorption Partition Coefficient, log $K_{OC}$:

- 1.85 (calculated-$K_{OW}$, Lyman et al. 1982)
- 0.64 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 0.50 (soil, quoted exptl., Meylan et al. 1992)
- 0.39 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 0.50 (calculated-$K_{OW}$, Kollig 1993)
- 0.50 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

- Volatilization: evaporation rate $k = 2.538 \times 10^{-4}$ mol m$^{-2}$ h$^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1)$ L h$^{-1}$ at 20 $\pm$ 0.1°C (Gückel et al. 1973);
  estimated half-lives, $t_{1/2} \sim$2.4 h in streams, $t_{1/2} \sim$3.9 h in rivers and $t_{1/2} \sim$125.9 h in lakes (Lyman et al. 1982; quoted, Howard 1990).

- Photolysis:
  Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$, with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
  
  $k = 2.2 \times 10^{9}$ L mol$^{-1}$ s$^{-1}$ for the reaction with 1 $\times$ 10$^{-17}$ M hydroxyl radical in water with $t_{1/2}$ $\sim$1 yr (Anbar & Neta 1967; quoted, Howard 1990)
  photooxidation $t_{1/2} = 2602–104000$ h in water, based on measured rate constant for reaction with OH radical in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991)
  
  $k_{OH} = 6.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)
  photooxidation $t_{1/2} = 0.24–2.4$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
  $t_{1/2} = 6.5$ h for the vapor phase reaction with photochemically produced NO radical in the atmosphere (Dilling et al. 1976; quoted, Howard 1990)
  
  $k_{OH} = 4.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (Lyman et al. 1982)
  $k = 0.58 \pm 0.06$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2.0-6.0 and 20–23°C (Hoigné & Bader 1983)
  
  $k_{OH}(\text{calc}) = 6.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(\text{obs.}) = 7.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
  photooxidation $t_{1/2} = 8.8–87.7$ h in air, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)
  estimated half-life of 2.3 d for the vapor phase reaction with photochemically produced NO radical in the atmosphere (GEMS 1986; quoted, Howard 1990)
  
  $k_{OH}(\text{exptl}) = 7.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{OH}(\text{calc}) = 6.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
  
  $k_{OH} = (8.31 \pm 0.63) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)
  
  $k_{OH}(\text{exptl}) = 8.31 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k(\text{soln}) = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with OH radical in aqueous solution (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987b)
  
  $k_{OH} = 8.31 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k(\text{soln}) = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
  
  $k_{OH} = (7.2 - 8.31) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 292–296 K (review, Atkinson 1989)
  
  $k_{OH} = 8.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1990)
  
  $k_{OH} = (7.80 \pm 0.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (8.56 \pm 0.70) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
  
  $k_{OH}(\text{calc}) = 8.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

- Hydrolysis:
- Biodegradation:
  
  $t_{1/2}(\text{aq. aerobic}) = 24–168$ h, based on unacclimated freshwater grab sample data (Hammerton 1955) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);
  $k = 84.0$ mg COD g$^{-1}$ h$^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
t_{1/2}(aq. anaerobic) = 96–1296 h, based on acclimated screening test data (Chou et al. 1979; selected, Howard et al. 1991) and aqueous aerobic biodegradation half-life (Howard et al. 1991);
k(calc) = (0.959 ± 0.063) × 10^2 h^{-1} by activated sludge (Yonezawa & Urushigawa 1979)
k = 0.035–0.046 h^{-1} in 30 mg/L activated sludge after a time lag of 5-10 h (Urano & Kato 1986).

**Biotransformation:**

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

**Half-Lives in the Environment:**

- **Air:** \( t_{1/2} = 0.24-2.4 \) h 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);
- **photodecomposition** \( t_{1/2} = 6.5 \) h under simulated atmospheric conditions, with NO (Dilling et al. 1976);
- **Photolysis** \( t_{1/2} = 1.2 \) d for the atmospheric reaction with \( 1 \times 10^{-6} \) molecules/cm^3 of OH radical (Howard 1990);
- **photooxidation** \( t_{1/2} = 8.8-87.7 \) h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected Howard et al. 1991).

**Surface water:** \( t_{1/2} = 24-168 \) h, based on unacclimated freshwater grab sample data (Hammerton 1955; selected, Howard et al. 1991) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

**photooxidation** \( t_{1/2} = 2602-104000 \) h, based on measured rate constant for reaction with hydroxyl radicals in aqueous solution (Dorflman & Adams 1973; selected, Howard et al. 1991);

**estimated volatilization half-lives,** \( t_{1/2} = 2.4 \) h in streams, \( t_{1/2} = 3.9 \) h in rivers and \( t_{1/2} = 125.9 \) h in lakes (Lyman et al. 1982; quoted, Howard 1990).

**Groundwater:** \( t_{1/2} = 48-1296 \) h, based on estimated aqueous anaerobic 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 11.1.1.5.1**

**Reported aqueous solubilities of 1-butanol at various temperatures**

1.

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<tr>
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De Santis et al. 1976

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FIGURE 11.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-butanol.
### Table 11.1.1.5.2
Reported vapor pressures of 1-butanol at various temperatures and the coefficients for the vapor pressure equations

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

#### 1.

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<tr>
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<th>Butler et al. 1935 isoteniscope method</th>
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1-Butanol (n-butyl alcohol): vapor pressure vs. 1/T

![Graph showing vapor pressure versus reciprocal temperature for 1-butanol.](image)

**FIGURE 11.1.1.5.2** Logarithm of vapor pressure versus reciprocal temperature for 1-butanol.

**TABLE 11.1.1.5.3**

Reported Henry's law constants of 1-butanol at various temperatures and temperature dependence equations

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

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

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

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

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

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**Snider & Dawson 1985**

- **gas stripping-GC**
  - 0°C: 0.0873
  - 25°C: 0.800

**Kolb et al. 1992**

- **equilibrium headspace-GC**
  - 25°C: 0.800
  - 60°C: 11.64
  - 70°C: 19.81
  - 80°C: 29.69

*enthalpy of transfer: \( \Delta H/(\text{kJ mol}^{-1}) = 58.576 \)*

- eq. 2a: \( 1/K_{AW} \)
  - A: -10.2
  - B: 5234
FIGURE 11.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-butanol.
11.1.1.6  Isobutanol (i-Butyl alcohol)

- **Common Name**: Isobutanol
- **Synonym**: isobutyl alcohol, 2-methyl-1-propanol, i-butyl alcohol
- **Chemical Name**: isobutanol, isobutyl alcohol, 2-methyl-1-propanol
- **CAS Registry No**: 78-83-1
- **Molecular Formula**: C₄H₁₀O, (CH₃)₂CHCH₂OH
- **Molecular Weight**: 74.121
- **Melting Point (°C)**: –101.9 (Lide 2003)
- **Boiling Point (°C)**: 1087.89 (Lide 2003)
- **Density (g/cm³ at 20°C)**:
  - 0.8018 (Weast 1982–83)
  - 0.8016, 0.7978 (20°C, 25°C, Riddick et al. 1986)
- **Molar Volume (cm³/mol)**:
  - 92.5 (20°C, calculated-density)
  - 103.6 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, ΔH₉ᵤₛ (kJ/mol)**: 6.32 (Riddick et al. 1986)
- **Entropy of Fusion, ΔS₉ᵤₛ (J/mol K)**: 56 (estimated, Yalkowsky & Valvani 1980)
- **Fugacity Ratio at 25°C (assuming ΔS₉ᵤₛ = 56 J/mol K), F**: 1.0

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

- 100140 (18°C, shake flask-turbidity, Fühner 1924)
- 85000 (20°C, Seidell 1941)
- 75600 (shake flask-interferometry, Donahue & Bartell 1952)
- 94000 (shake flask-colorimetric, De Santis et al. 1976)
- 95000 (18°C, Verschueren 1983)
- 76270 (IUPAC recommended, Barton 1984)
- 100000 (Dean 1985; 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):**

- \( \log (P/\text{mmHg}) = 43.5513 - 4185/(T/K) - 11.50\log (T/K) \); temp range 25–100°C (isoteniscope measurements, Butler et al. 1935)
- 1648 (interpolated-regression of tabulated data, Stull 1947)
- 1333* (21.7°C, summary of literature data, temp range –9.0 to 108°C, Stull 1947)
- 1527* (comparative ebulliometry, measured range 343.044–388.733 K, Ambrose & Sprake 1970)
- \( \log (P/\text{mmHg}) = [–0.2185 \times 10936.0/(T/K)] + 9.1138032 \); temp range –9.0 to 241°C (Antoine eq., Weast 1972–73)
- 1527 (selected, Riddick et al. 1986)
- \( \log (P/\text{kPa}) = 6.50091 - 1295.197/(T/°C + 175.787) \), temp range not specified (Riddick et al. 1986)
- \( \log (P/\text{kPa}) = 6.34528 - 1190.463/(–106.712 + T/K) \); temp range 369–389 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\[ \log (P_{\text{L}}/\text{kPa}) = 6.49241 - 1271.027/(–97.758 + T/\text{K}); \text{ temp range 313–411 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]
\[ \log (P_{\text{L}}/\text{kPa}) = 7.05055 - 1511.48/(–81.634 + T/\text{K}); \text{ temp range 381–524 K (Antoine eq.-III, Stephenson & Malanowski 1987)} \]
\[ \log (P_{\text{L}}/\text{kPa}) = 9.8507 - 2875/(T/\text{K}); \text{ temp range 202–243 K (Antoine eq.-IV, Stephenson & Malanowski 1987)} \]
\[ \log (P_{\text{L}}/\text{kPa}) = 6.34606 - 1190.8481/(–106.673 + T/\text{K}); \text{ temp range 369–389 K (Antoine eq.-V, Stephenson & Malanowski 1987)} \]
\[ \log (P_{\text{L}}/\text{kPa}) = 6.50104 - 1275.669/(–97.269 + T/\text{K}); \text{ temp range 342–389 K (Antoine eq.-VI, Stephenson & Malanowski 1987)} \]
\[ \log (P_{\text{L}}/\text{kPa}) = 6.27047 - 1147.676/(–111.933 + T/\text{K}); \text{ temp range 383–416 K (Antoine eq.-VII, Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 109.2803 - 6.306 \times 10^3/(T/\text{K}) - 36.947 \cdot \log(T/\text{K}) + 1.4462 \times 10^{-2} \cdot (T/\text{K}) - 3.948 \times 10^{-13} \cdot (T/\text{K})^2; \text{ temp range 165–548 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa·m^3/mol at 25°C):
1.20 (measured partial pressure/mole fraction \( x \) at dilute concn, Butler et al. 1935)
1.214 (exptl.-C\( _W/c_{CA} \), Hine & Mookerjee 1975)
1.159, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.992 (headspace-GC, Snider & Dawson 1985)
1.186 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988b)
1.84 (solid-phase microextraction SPME-GC, Bartelt 1997)
2.73 (gas stripping-GC, Shiu & Mackay 1997)
0.892 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
0.83 (shake flask-CR, Collander 1951)
0.61 (calculated-\( \pi \) constant, Hansch et al. 1968)
0.64 (Leo et al. 1969)
0.65 (from Hansch & Dunn III unpublished result, Leo et al. 1971)
0.76 (shake flask-GC, Dillingham et al. 1973)
0.76 (shake flask, Hansch & Leo 1985; 1987)
0.76 (recommended, Sangster 1989, 1993)
0.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):
3.80 (calculated-measured \( \gamma \) in pure octanol and vapor pressure \( P \), Abraham et al. 2001)

Bioconcentration Partition Factor, log BCF:

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

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

Volatileization: using Henry’s law constant, \( t_{1/2}(\text{calc}) = 79.7 \text{ h for evaporation from a model river of 1-m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).} \)

Photolysis:

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

photooxidation \( t_{1/2} = 201 \text{ d to 22 yr in water, based on measured rate for the reaction with OH radical in water (Anbar & Neta 1967; selected, Howard et al. 1991) \}

photooxidation \( t_{1/2} = 0.24–2.4 \text{ h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976) \} \)
Alcohols

photooxidation $t_{1/2} = 9.96–99.6$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:
Biodegradation: biodegradation rate constant $k = 0.015–0.020$ h$^{-1}$ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986)

- $t_{1/2}$(aq. aerobic) = 43–173 h, based on river die-away data for one sample of water from one river (Hammerton 1955; selected, Howard et al. 1991)
- $t_{1/2}$(aq. anaerobic) = 172–692 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 half-life of 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition $t_{1/2} = 3.5$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976);
- photooxidation $t_{1/2} = 9.96–99.6$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

- Surface water: photooxidation $t_{1/2} = 201$ d to 22 yr, based on measured rate for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2} = 43–173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

- Groundwater: $t_{1/2} = 86–346$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

- Soil: $t_{1/2} = 43–173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

- biota:

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<td>Reported vapor pressures of isobutanol at various temperatures and the coefficients for the equations</td>
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FIGURE 11.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for isobutanol.
### sec-Butyl alcohol

**Common Name:** sec-Butyl alcohol  
**Synonym:** 2-butyl alcohol, 2-butanol, methylethylcarbinol  
**Chemical Name:** 2-butanol, sec-butyl alcohol  
**CAS Registry No:** 78-92-2  
**Molecular Formula:** C₄H₁₀O, CH₃CH₂CHOHCH₃  
**Molecular Weight:** 74.121

- **Melting Point (°C):** -88.5 (Lide 2003)  
- **Boiling Point (°C):** 99.51 (Lide 2003)  
- **Density (g/cm³ at 20°C):** 0.8063 (Weast 1982–83)  
  0.8065, 0.8024 (20°C, 25°C, Riddick et al. 1986)  
- **Molar Volume (cm³/mol):** 91.9 (20°C, calculated-density)  
  103.6 (calculated-Le Bas method at normal boiling point)  
- **Enthalpy of Fusion, ΔH_{fus} (kJ/mol):** 56 (estimated, Yalkowsky & Valvani 1980)  
- **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. Additional data at other temperatures designated * are compiled at the end of this section):**  
  200000 (20°C, synthetic method, Jones 1929)  
  185000 (20°C, shake flask, Evans 1936)  
  198000* (20°C, shake flask-refractometer, measured range 20–85°C, Morachevskii & Popovich 1965)  
  177000, 165000 (25, 35°C, shake flask-titration, Ratouis & Dodé 1965)  
  202000* (20°C, equilibrium pressure cell/shake flask-refractometric method, measured range 10–110°C, pressure range 1–800 atm, Moriyoshi et al. 1975)  
  225000 (shake flask-colorimetric analysis, De Santis et al. 1976)  
  130000 (shake flask-refractometric method, Becke & Quitzch 1977)  
  187000* (equilibrium pressure vessel/shake flask-GC, measured range 265–372 K, pressure range 0.1–75 MPa, Bozdag & Lamb 1983)  
  181000* (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)  
  196000* (20°C, shake flask-GC/TC, measured range 0–90.2°C, Stephenson & Stuart 1986)  
  175340* (25.28°C, shake flask-laser scattering technique, measured range 276.94–386.6 K, Ochi et al. 1996)

**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):**  
  2286* (modified isoteniscope method, measured range 25–91°C. Butler et al. 1935)  
  log (P/mmHg) = 43.4800– 4110/(T/K) – 11.50-log (T/K); temp range 25–90°C (isoteniscope measurements, Butler et al. 1935)  
  2266* (interpolated-regression of tabulated data, temp range –12.2 to 99.5°C, Stull 1947)  
  33031* (73.392°C, ebulliometry, measured range 73.392–107.146°C, Biddiscombe et al. 1954)  
  log (P/Pa) = 6.26852 – 1126.667/(T/K – 108.361); restricted temp range 67.7–83.34°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)  
  log (P/Pa) = 6.86618 – 1360.131/(T/K – 75.558); temp range 67.723–107.743°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
log (P/mmHg) = \[-0.2185 \times 10^{712.3/(T/K)}\] + 9.096778; temp range -12.2–251°C (Antoine eq., Weast 1972–73)

1600, 3200 (20°C, 30°C, Verschueren 1983)

2200, 2190, 2275 (extrapolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.35079 – 1169.924/(169.731 + t°C); temp range 67.7–107.14°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 6.26823 – 1126.887/(–108.291 + T/K); temp range 359–381 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P/kPa) = 6.34976 – 1169.754/(–103.388 + T/K); temp range 303–403 K (Antoine eq-II., Stephenson & Malanowski 1987)

log (P/kPa) = 5.74369 – 735.87/(–176.795 + T/K); temp range 372–5241 K (Antoine eq-III., Stephenson & Malanowski 1987)

log (P/kPa) = 7.50959 – 1751.931/(–52.906 + T/K); temp range 210–303 K (Antoine eq-IV., Stephenson & Malanowski 1987)

log (P/kPa) = 6.2663 – 1125.853/(–108.414 + T/K); temp range 359–380 K (Antoine eq-V., Stephenson & Malanowski 1987)

log (P/kPa) = 6.35314 – 1171.484/(–103.199 + T/K); temp range 340–379 K (Antoine eq-VI., Stephenson & Malanowski 1987)

log (P/mmHg) = 49.4476 – 4.2487 × 10^3/(T/K) – 13.793 · log(T/K) + 6.2736 × 10^{-11} · (T/K)^2; temp range 158–536 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. Additional data at other temperatures designated * are compiled at the end of this section):

1.040 (measured partial pressure/mole fraction x at dilute concn, Butler 1935)

1.033 (exptl., Hine & Mookerjee 1975)

1.60, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.918* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

1.107 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988b)

0.604 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log \( K_{AW} \) = 6.734 – 3031/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.61 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)

0.74, 0.64 (calculated-f const., calculated-\( \pi \) const., Rekker 1977)

0.81 (HPLC-RT correlation, Yonezawa & Urushigawa 1979)

0.87 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)

0.65 (recommended, Sangster 1989)

0.61 (recommended, Hansch et al. 1995)

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

3.99* (20.29°C, from GC determined \( \gamma \) in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

3.80 (calculated from determined \( \gamma \) in octanol and vapor pressure, Abraham et al. 2001)
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, k<sub>OH</sub> for reaction with OH radical, k<sub>NO3</sub> with NO₃ radical and k<sub>O3</sub> with O₃ or as indicated, *data at other temperatures see reference:

photooxidation t<sub>½</sub> = 129 d to 23 yr, based on measured rate for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation t<sub>½</sub> = 0.24–2.4 h 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)

k < 2 × 10<sup>2</sup> M<sup>–1</sup> s<sup>–1</sup> for oxidation by singlet oxygen at 25°C in aquatic systems with t<sub>½</sub> > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)

k<sub>OH</sub> = 4.1 × 10<sup>9</sup> M<sup>–1</sup> s<sup>–1</sup> for at 25°C with t<sub>½</sub> = 1.3 d (Hendry & Kenley 1979; quoted, Mill 1982)

**Hydrolysis:**

**Biodegradation:**

aqueous aerobic t<sub>½</sub> = 24–168 h, based on river die-away studies (Hammerton 1955; selected, Howard et al. 1991) and aqueous anaerobic t<sub>½</sub> = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (selected, Howard et al. 1991);

average rate of biodegradation k<sub>B</sub> = 55.0 (mg COD g<sup>–1</sup> h<sup>–1</sup>) based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

**Biotransformation:**

**Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:**

Half-Lives in the Environment:

Air: photooxidation t<sub>½</sub> = 0.24–2.4 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition t<sub>½</sub> = 4.0 h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

photooxidation t<sub>½</sub> = 7.2–72 h, based on measured rate constant for the reaction with OH radical in air (Edney & Corse 1986; selected, Howard et al. 1991);

calculated lifetimes of 1.3 d and 17 d for reactions with OH radical, NO₃ radical, respectively (Atkinson 2000)

Surface water: t<sub>½</sub> = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: t<sub>½</sub> = 48–336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: t<sub>½</sub> = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

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**TABLE 11.1.1.7.1**

**Reported aqueous solubilities of sec-butyl alcohol at various temperatures**

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pressure range 1–800 atm
full list of data see ref.

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Alcohols

FIGURE 11.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for sec-butyl alcohol.

<table>
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TABLE 11.1.1.7.2
Reported vapor pressures of sec-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

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

1. Butler et al. 1935
   Stull 1947
   Biddiscombe et al. 1954
   Brown et al. 1969

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<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>99.410</td>
<td>101321</td>
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\[\text{eq. 4:} \quad P/mmHg = 120.611 \quad 113533\]
\[A = 43.4800 \quad 120.186 \quad 120168\]
\[B = 4110 \quad 105.647 \quad 126596\]
\[C = 11.50 \quad 107.146 \quad 133.471\]

\[\Delta H/_c/(kJ \text{ mol}^{-1}) = 50.21 \quad \text{at} \quad 25°C\]

(Continued)
2. Ambrose & Sprake 1970 comparative ebulliometry

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**FIGURE 11.1.1.7.2** Logarithm of vapor pressure versus reciprocal temperature for sec-butyl alcohol.
TABLE 11.1.1.7.3
Reported Henry's law constants and octanol-air partition coefficients of sec-butyl alcohol at various temperatures

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log ( K_{OA} )</th>
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</thead>
<tbody>
<tr>
<td>Snider &amp; Dawson 1985</td>
<td></td>
</tr>
<tr>
<td>gas stripping-GC</td>
<td></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( H/(Pa m^3/mol) )</td>
</tr>
<tr>
<td>0</td>
<td>0.0987</td>
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<tr>
<td>25</td>
<td>0.9180</td>
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<tr>
<td>enthalpy of transfer:</td>
<td>( \Delta H/(kJ mol^{-1}) = 58.576 )</td>
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</table>

FIGURE 11.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for sec-butyl alcohol.

FIGURE 11.1.1.7.4 Logarithm of \( K_{OA} \) versus reciprocal temperature for sec-butyl alcohol.
11.1.1.8 tert-Butyl alcohol

Common Name: tert-Butyl alcohol
Synonym: 3-butanol, t-butyl alcohol, 2-methyl-2-propanol, trimethylcarbinol,
Chemical Name: t-butanol, t-butyl alcohol, 2-methyl-2-propanol
CAS Registry No: 75-65-0
Molecular Formula: C₄H₁₀O, (CH₃)₃COH
Molecular Weight: 74.121
Melting Point (°C):
25.69 (Lide 2003)
Boiling Point (°C):
82.4 (Lide 2003)
Density (g/cm³ at 20°C):
0.78581, 0.78086 (20°C, 25°C, Dreisbach & Martin 1949)
0.7883 (Weast 1982–83)
0.7858 (Dean 1985)
0.7812 (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
94.2 (calculated-density, Rohrschneider 1973)
103.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHfus (kJ/mol):
6.64 (Riddick et al. 1986)
Entropy of Fusion, ΔSfus (J/mol K):
22.76, 56 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
miscible (Palit 1947; Riddick et al. 1986)
miscible (Barton 1984; Dean 1985; Howard 1990; Yaws et al. 1990)
miscible (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):
5600* (static method/isotenoscope, measured range 20–90°C, Parks & Barton 1928)
log (P/mmHg) = 43.2834 – 3935/(T/K) –11.50-log (T/K); temp range 30–80°C (isotenoscope measurements,
Butler et al. 1935)
5019* (interpolated-regression of tabulated data, temp range –20.4 to 82.9°C, Stull 1947)
log (P/mmHg) = 8.24380 – 1675.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
16500* (43.34°C, measured range 43.34–82.41°C, Dreisbach & Shrader 1949)
log (P/Pa) = 6.35648 – 1107.060/(T/K – 101.048); temp range 329.946–362.71 K (Antoine eq.,
comparative ebulliometry, Ambrose & Sprake 1970)
log (P/Pa) = 6.35648 – 1107.060/(T/K – 101.048); temp range 329.946–362.71 K (Antoine eq.,
comparative ebulliometry, Ambrose & Sprake 1970)
log (P/mmHg) = [–0.2185 × 10413.2/(T/K)] + 9.193472; temp range –20.4 to 222.5°C (Antoine eq., Weast
1972–73)
5600 (Verschueren 1983; Howard et al. 1986)
5637 (selected, Riddick et al. 1986)
log (P/kPa) = 6.35648 – 1107.060/(373 + 172.102) temp not specified (Riddick et al. 1986)
log (P/Pa) = 6.22619 – 1042.416/(–108.5 + T/K); temp range 347–363 K (Antoine eq.-I, Stephenson &
Malanowski 1987)
Alcohols

log \( P \text{L}/\text{kPa} \) = 6.35045 – 1104.341/\((-101.315 + T/\text{K})\); temp range 299–375 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( P \text{L}/\text{kPa} \) = 6.27388 – 989.74/(–124.966 + T/\text{K}); temp range 356–480 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log \( P \text{L}/\text{kPa} \) = 6.23125 – 1044.891/(–108.211 + T/\text{K}), temp range: 347–363 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)

log \( P \text{L}/\text{kPa} \) = 6.35498 – 1106.556/(–101.071 + T/K); temp range 329–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log \( P \text{L}/\text{kPa} \) = 6.09542 – 975.944/(–116.864 + T/K); temp range 357–461 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

\( \log (P/\text{mmHg}) = 71.8181 – 4.9966 \times 10^3/(T/\text{K}) – 21.805 \times \log (T/\text{K}) + 1.9238 \times 10^{-8} \times (T/\text{K})^2; \) temp range 299–506 K (vapor pressure eq., Yaws 1994)

log \( P \text{L}/\text{kPa} \) = 1008, 5600 (calculated-solvatochromic parameters, quoted lit., Banerjee et al. 1990)

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):

1.210 (measured partial pressure/mole fraction \( x \) at dilute concn, Butler et al. 1935)

1.214 (exppl., Hine & Mookerjee 1975)

1.057, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.460* (25°C headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

1.426 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988b)

0.917 (wetted-wall chromatographic GC, Altschuh et al. 1999)

0.907 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

\( \log K_{\text{AW}} = 8.467 – 3488/(T/\text{K}) \) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.37 (shake flask–GC, Hansch & Anderson 1967; Leo et al. 1969)

0.59 (HPLC–RT correlation, Yonezawa & Urushigawa 1979)

0.35 (Hansch & Leo 1985)

0.40 (calculated-solvatochromic parameters, Taft et al. 1985)

0.39 (HPLC–k′ correlation, Funasaki et al. 1986)

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

0.35 (recommended, Sangster 1989)

0.34 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)

0.35 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, \( BCF \):

-1.46 (calculated-\( K_{\text{ow}} \), Lyman et al. 1982; quoted, Howard 1990)

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

1.57 (soil, calculated-\( K_{\text{ow}} \), Lyman et al. 1982; quoted, Howard 1990)

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

Volutilization: estimated half-lives, \( t_{1/2} \) = 51.6 h in streams, \( t_{1/2} \) = 65.37 h in rivers and \( t_{1/2} \) = 3104.3 h in lakes were estimated by using Henry’s law constant and assuming the wind velocity to be 3 m/s, the current velocities of the streams, rivers, and lakes 2.1, and 0.01 m/s with depths of lakes 50 m and that of the streams and lakes 1 m deep (Lyman et al. 1982; quoted, Howard 1990).

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

- photoxidation $t_{1/2} = 771$ d to 64500 yr, based on measured rate for the reaction with hydroxyl radical in water (Howard et al. 1991)
- photoxidation $t_{1/2} > 9.9$ d (Darnall et al. 1976)
- $k \sim 0.003$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2–6 and 20–23°C (Hoigné & Bader 1983)
- $k_{OH}(\text{calc}) = 6.9 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(\text{obs.}) = 1.09 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)
- photoxidation $t_{1/2} = 59$–590 h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)
- $k_{OH}(\text{calc}) = 5.9 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{OH}(\text{exptl}) = 1.09 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
- $k_{OH} = (1.08 \pm 0.11) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)
- $k_{OH} = 1.07 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k(\text{soln}) = 1.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
- $k_{OH} = 1.07 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 243–440 K (flash photolysis-resonance fluorescence, Wallington 1988c)
- $k_{OH} = 1.12 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
- $k(\text{aq.}) = 0.01$ M$^{-1}$ s$^{-1}$ at pH 2.3, $k = 0.45$ M$^{-1}$ s$^{-1}$ at pH 2.2, $k = 0.46$ M$^{-1}$ s$^{-1}$ at pH 5.2 for direct reaction with ozone in water and 20°C, with $t_{1/2} = 390$ d at pH 7 (Yao & Haag 1991).
- $k_{OH}(\text{calc}) = 0.53 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation 30.0 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

- $t_{1/2}(\text{aerobic}) = 677$–4320 h, based on river die-away studies; $t_{1/2}(\text{anaerobic}) = 2400$–12000 h, based on degradation rates in microcosm studies simulating anaerobic aquifers (Howard et al. 1991).
- $t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 100$ d in natural waters (Capel & Larson 1995)

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

Half-Lives in the Environment:

Air: photoxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

- $t_{1/2} = 34.5$ h for 10 ppm in the air reacted with 5 ppm NO (Dilling et al. 1976);
- photoxidation $t_{1/2} = 59$–590 h, based on measured rate for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);
- $t_{1/2} \sim 1.09$ month for the vapor phase reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2} \sim 8.8$ yr, based on rate constant $k = 2.5 \times 10^9$ L/mol·s for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard 1990);

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

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

Sediment:

- Soil: $t_{1/2} = 360$–4800 h, based on soil microcosm studies (Howard et al. 1991).

Biota:
### TABLE 11.1.1.8.1
Reported vapor pressures of tert-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

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

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<th>Isoteniscope method</th>
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<th>Comparative ebulliometry</th>
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</table>

\[\Delta H_v/(kJ \text{ mol}^{-1}) = \Delta H_v/(kJ \text{ mol}^{-1}) = 46.86\]

<table>
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FIGURE 11.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for tert-butyl alcohol.

TABLE 11.1.1.8.2
Reported Henry’s law constants of tert-butyl alcohol at various temperatures

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<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
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<td>0</td>
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<td>1.4581</td>
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enthalpy of transfer:
\[ \Delta H/(\text{kJ mol}^{-1}) = 66.944 \]

FIGURE 11.1.1.8.2 Logarithm of Henry’s law constant versus reciprocal temperature for tert-butyl alcohol.
11.1.1.9  1-Pentanol (n-Amyl alcohol)

Common Name: 1-Pentanol
Synonym: amyl alcohol, n-butylcarbinol, 1-pentanol, n-pentyl alcohol, pentyl alcohol
Chemical Name: n-amyl alcohol, n-pentyl alcohol, 1-pentanol
CAS Registry No: 71-41-0
Molecular Formula: C₅H₁₂O, CH₃CH₂CH₂CH₂CH₂OH
Molecular Weight: 88.148
Melting Point (°C): 
  –77.6  (Lide 2003)
Boiling Point (°C):
  137.98  (Lide 2003)
Density (g/cm³ at 20°C):
  0.81253  (25°C, Butler et al. 1935)
  0.8144  (Weast 1982–83)
  0.81445, 0.81080  (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  108.0  (calculated-density, Lande & Banerjee 1981)
  125.8  (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
  20.81  (Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₘₚ (kJ/mol):
  10.5  (Riddick et al. 1986)
Entropy of Fusion, ∆Sₘₚ (J/mol K):
  56  (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ∆Sₘₚ = 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):
  22080  (shake flask-interferometer, Butler et al. 1933)
  21900*  (volumetric method, measured range 20–30°C, Ginnings & Baum 1937)
  22100  (20°C, surface tension, Addison 1945)
  23600  (20°C, Seidell 1941)
  27570  (shake flask-residue volume, Booth & Everson 1948)
  15230  (20°C, shake flask-turbidity, Laddha & Smith 1948)
  25400  (shake flask-interferometry, Hansen et al. 1949)
  23500*  (20°C, synthetic method, measured range 0–180°C, von Erichsen 1952)
  22000  (shake flask-titration, Crittenden & Hixon 1954)
  22140  (estimated, McGowan 1954)
  22000  (surface tension, Kinoshita et al. 1958)
  23800  (shake flask-GC, Korenman 1974, 1975)
  21950  (Riddick & Bunger 1955)
  18800  (shake flask-GC, Evans et al. 1978)
  11720  (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
  22000*  (recommended best value, IUPAC Solubility Data Series, temp range 0–180°C, Barton 1984)
  22500*  (20.2°C, shake flask-GC/TC, measured range 0–90.7°C, Stephenson et al. 1984)
  20190  (shake flask-GC, Li & Andren 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):
**Henry’s Law Constant (Pa m³/mol):**

1.324 (measured partial pressure/mole fraction \( x \) at dilute concn, Butler et al. 1935)

1.271 (exptl., Hine & Mukherjee 1975)

1.426, 1.60 (calculated-group contribution, calculated-bond contribution, Hine & Mukherjee 1975)

1.04 (calculated-P/C, Mackay & Yuen 1983)

1.017 (limiting activity coefficient by headspace-GC, Abraham et al. 1987)

1.271 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988)

1.236 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

1.60 (correlated-molecular structure, Russell et al. 1992)

1.186 (limiting activity coefficient by headspace-GC, Li & Carr 1993)

1.057 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

\[
\ln K_{AW} = 14.233 - 6559.6/(T/K); \text{ temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)}
\]

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

1.40 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Dunn III 1972)
1.37, 1.38, 1.34 (calculated-fragment const.; calculated-$\pi$ constant, Rekker 1977)
1.44, 1.48 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
1.53 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
1.33 (HPLC-RT correlation, D’Amboise & Hanai 1982)
1.56 (shake flask, Log P Database, Hansch & Leo 1987)
1.49 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
1.53 (generator column-GC, Schantz & Martire 1987)
1.55 (calculated from measured $\gamma$, Schantz & Martire 1987)
1.51 (recommended value, Sangster 1989, 1993)
1.41 (shake flask-GC, Fujiwara et al. 1991)
1.56 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
0.241 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log $K_{OC}$:
0.93 (calculated-MCI $\chi$, Gerstl & Helling 1987)
0.70 (soil, quoted exp., Meylan et al. 1992)
0.65 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
0.70 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization: evaporation rate of $6.92 \times 10^{-5}$ mol cm$^{-2}$ h$^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1)$ L h$^{-1}$ at $20 \pm 0.1^\circ$C (Gückel et al. 1973).

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference: photooxidation $t_{1/2} = 0.24–2.4$ h 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)

$k_{OH}(\text{exptl}) = 1.08 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k = 6.50 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with hydroxyl radical in aqueous solution at 298 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987)
$k_{OH} = 1.08 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k(\text{soln}) = 6.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 10.8 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (review, Atkinson 1989)
$k_{OH} = (12.0 \pm 1.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (10.5 \pm 1.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ by relative rate method, at 298 $\pm$ 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 9.37 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

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

Half-Lives in the Environment:
Air: $t_{1/2} = 0.24–2.4$ h 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).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:
### TABLE 11.1.9.1
Reported aqueous solubilities of 1-pentanol at various temperatures

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**FIGURE 11.1.9.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-pentanol.
TABLE 11.1.1.9.2
Reported vapor pressures of 1-pentanol at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

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<td>∆Hv/(kJ mol⁻¹) = 56.90</td>
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Antoine eq. for full range

eq. 3 P/mmHg

A 6.30306
B 1286.333
C 111.843

Data also fitted to Cragoe equation, see ref.
FIGURE 11.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1-pentanol.
11.1.1.10 1-Hexanol

Common Name: 1-Hexanol
Synonym: amylcarbinol, 1-hexanol, n-hexyl alcohol
Chemical Name: n-hexyl alcohol, 1-hexanol
CAS Registry No: 111-27-3
Molecular Formula: C₆H₁₄O, CH₃CH₂CH₂CH₂CH₂CH₂OH
Molecular Weight: 102.174

Melting Point (°C):
-47.4 (Lide 2003)

Boiling Point (°C):
157.6 (Lide 2003)

Density (g/cm³ at 20°C):
0.8136 (Weast 1982–83)
0.81875, 0.81534 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
126.0 (calculated-density, Lande & Banerjee 1981)
148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_fus (kJ/mol):
15.40 (Riddick et al. 1986)

Entropy of Fusion, ΔS_fus (J/mol K):
56 (estimated, Yalkowsky & Valvani 1980)

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. Additional data at other temperatures designated * are compiled at the end of this section):
5000* (20°C, shake flask-turbidity, measured range 0–110°C, Fühner 1924)
6240 (shake flask-interferometer, Butler et al. 1933)
5025 (20°C, shake flask-turbidity, Laddha & Smith 1948)
6400* (20°C, synthetic method, measured range 0–220°C, von Erichsen 1952)
6000 (shake flask-titration, Crittenden & Hixon 1954)
6300 (estimated, McGowan 1954)
6000 (surface tension, Kinoshita et al. 1958)
5838* (shake flask-refractive index, measured range 5.5–33.6°C, Hill & White 1974)
3590 (shake flask-GC, Korenman et al. 1974)
4230 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
6000* (recommended best value, IUPAC Solubility Series, temp range 0–220°C, Barton 1984)
6600* (20°C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson et al. 1984)
5354 (shake flask-GC, Li & Andren 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):
95.86* (24.98°C, extrapolated-modified isoteniscope data, measured range 60.11–152.77°C, Butler et al. 1935)
log (P/mmHg) = 51.0030 – 5068/(T/K) – 13.80·log (T/K), temp range 60–152°C (isoteniscope measurements, Butler et al. 1935)
151.1* (interpolated-regression of tabulated data, temp range 24.4–157°C, Stull 1947)
88.25 (extrapolated, ebulliometry, measured range 52–157°C, Kemme & Kreps 1969)
760* (52.2°C, ebulliometry-differential thermal analysis, measured range 52.3–157.3°C, Kemme & Kreps 1969)
log (P/mmHg) = –0.2185 × 12708.5/(T/°C) + 9.367617; temp range 24.4–157°C (Antoine eq., Weast 1972–73)
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130.6 (20°C, Verschueren 1983)
79.65, 79.7 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.20107 – 1305.63/(153.901 + t°C); temp range 52.2–157.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.23614 – 1334.63/(156.297 + t°C); temp range 60.11–152.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
55.5 (extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
52.9, 254, 888 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)
109.5 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.86045 – 1707.26/(196.66 + t°C); temp range 35–157°C (Antoine eq., Dean 1985, 1992)
110 (selected, Riddick et al. 1986)
log (P/kPa) = 4.14271 – 1422.031/(t°C + 165.444); temp range not specified (Riddick et al. 1986)
111 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 4.14271 – 1422.031/(-107.706 + T/K); temp range 325–431 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 10.60355 – 3986.406/(46.713 + T/K); temp range 298–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 53.9686 – 4.9501 × 10^3/(T/K) – 15.199·log(T/K) + 2.3647 × 10^6·(T/K)^2; temp range 229–611 K (vapor pressure eq., Yaws 1994)
113* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)
ln (P/kPa) = 8.472727 – 1275.055/(T/K – 178.568); temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

Henry’s Law Constant (Pa m^3/mol at 25°C):
1.562 (measured partial pressure/mole fraction x at dilute aqueous solution, Butler et al. 1935)
1.735 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
1.562 (exptl., Hine & Mookerjee 1975)
1.88, 2.367 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1.46 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
1.60 (calculated-MCI γ, Nirmalakhandan & Speece 1988b)
1.896 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1.56 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
1.016 (wetted-wall column-GC, Altschuh et al. 1999)
2.60 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
ln K_{AW} = 11.705 – 5538.7/(T/K); temp range 40–90°C (van’t Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
2.03 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Dunn III 1972)
1.99 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
2.03 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
1.86 (RP-HPLC-k’ correlation, D’Amboise & Hanai 1982)
2.03 (HPLC-k’ correlation, Funasaki et al. 1986)
2.04 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
2.03 (generator column-GC, Schantz & Martire 1987)
2.05 (calculated from measured γ, Schantz & Martire 1987)
1.50 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
2.03 (recommended, Sangster 1989, 1993)
2.03 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
0.711 (calculated as per Mackay 1982, Schultz et al. 1990)
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Sorption Partition Coefficient, log $K_{OC}$:
- 1.01 (soil, quoted exptl., Meylan et al. 1992)
- 0.92 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 1.01 (calculated-MCI $\chi$, Sabljic et al. 1995)

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

Volatilization: evaporation rate of $1.85 \times 10^{-5}$ mol·cm⁻²·h⁻¹ was determined by gravimetric method with an airflow rate of $(50 \pm 1)$ L·h⁻¹ at $(20 \pm 0.1){}^\circ$C (Gückel et al. 1973).

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 $t_\frac{1}{2} = 0.24$–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).
- $k_{OH(\text{exptl})} = (12.4 \pm 0.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH(\text{calc})} = 10.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a).
- $k_{OH(\text{exptl})} = 1.24 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K, and $k(\text{soln}) = 1.20 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for the reaction with OH radical in aqueous solution (Wallington et al. 1988b).
- $k_{OH} = 12.4 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1989).
- $k_{OH} = (12.2 \pm 2.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy; $k_{OH} = (12.9 \pm 1.2) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ by relative rate method, at 298 ± 2 K (Nelson et al. 1990).
- $k_{OH(\text{calc})} = 10.48 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_\frac{1}{2} = 0.24$–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota

**TABLE 11.1.1.10.1**

Reported aqueous solubilities of 1-hexanol at various temperatures

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(Continued)
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2.

**Stephenson et al. 1984**

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Alcohols

FIGURE 11.1.1.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-hexanol.

TABLE 11.1.1.10.2
Reported vapor pressures of 1-hexanol at various temperatures and the coefficients for the vapor pressure equations

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

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<td>differential thermal analysis</td>
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<td>$t/°C$</td>
<td>P/Pa</td>
<td>$t/°C$</td>
<td>P/Pa</td>
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bp/°C | 155.7 |
D$^{25}$ | 0.8183 |

\begin{align*}
\text{bp/°C} &= 144.5 \\
\text{D}_{25} &= 157.3
\end{align*}

\begin{align*}
\Delta H_m/(kJ mol^{-1}) &= 62.84 \\
\text{at 25°C}
\end{align*}

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FIGURE 11.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexanol.
11.1.1.11 1-Heptanol

Common Name: 1-Heptanol
Synonym: 1-heptanol, n-heptyl alcohol
Chemical Name: n-heptyl alcohol, 1-heptanol
CAS Registry No: 111-70-6
Molecular Formula: C₇H₁₆O, CH₃(CH₂)₆OH
Molecular Weight: 116.201
Melting Point (°C): 
   –33.2 (Lide 2003)
Boiling Point (°C): 
   176.45 (Lide 2003)
Density (g/cm³ at 20°C): 
   0.82053 (25°C, Butler et al. 1935)
   0.8219 (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol): 
   142.0 (calculated-density, Lande & Banerjee 1981)
   170.2 (calculated- Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol): 
   56 (estimated, Yalkowsky & Valvani 1980)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K): 
   1740* (recommended best value, IUPAC Solubility Data Series, temp range 0–240°C, Barton 1984)
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 and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   930* (18°C, shake flask-turbidity, measured range 70–130°C, Fühner 1924)
   1804 (shake flask- interferometer, Butler et al. 1933)
   1720 (20°C, shake flask-titration, Addison 1943)
   3288 (shake flask-centrifuge, Booth & Everson 1948)
   1200 (shake flask-turbidimetric method, Harkins & Oppenheimer 1949)
   2000* (20°C, synthetic method, measured range 0–245°C, von Erichsen 1952)
   1800 (estimated, McGowan 1954)
   1700 (surface tension, Kinoshita et al. 1958)
   1500* (20°C, surface tension, 15–60 °C, measured range Vochten & Petre 1973)
   1676* (shake flask-interferometric method, measured range 6–34.9°C, Hill & White 1974)
   1313 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
   1740* (recommended best value, IUPAC Solubility Data Series, temp range 0–240°C, Barton 1984)
   1840* (20.2°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson et al. 1984)
   1510 (shake flask-GC, Li & Andren 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):
   29.86* (extrapolated, modified isoteniscope method, measured range 60–110°C, Butler et al. 1935)
   \[ \log (P/\text{mmHg}) = 55.1972 - 5580/(T/K) - 15.41 \log (T/K); \text{ temp range 60–152°C (isoteniscope measurements, Butler et al. 1935)} \]
   44.04* (extrapolated-regression of tabulated data, temp range 42.4–175.8°C, Stull 1947)
   22.2 (extrapolated-Antoine eq., ebulliometry, Kemme & Kreps 1969)
   626.6* (63.5°C, ebulliometry-differential thermal analysis, measured range 63.6–176.4°C, Kemme & Kreps 1969)
   \[ \log (P/\text{mmHg}) = 6.85450 - 1266.783/(139.663 + t/°C); \text{ temp range 63.6–176.4°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)} \]
   31.30 (calculated-Antoine eq., Jordan 1970)
   \[ \log (P/\text{mmHg}) = [-0.2185 \times 13920.9/(T/K)] + 9.720613; \text{ temp range 42.4–175.8°C (Antoine eq., Weast 1972–73)} \]
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12.8 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

24.0 (extrapolated-Antoine eq., Boublík et al. 1984)

\[ \log (P/kPa) = 6.10824 - 1323.566/(146.241 + t/°C); \text{ temp range 63.6–176.4°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)} \]

\[ \log (P/kPa) = 6.01857 - 1278.78/(146.403 + t/°C); \text{ temp range 60.11–152.8°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)} \]

17.64 (extrapolated-Antoine eq., Dean 1985)

\[ \log (P/mmHg) = 6.64767 - 1140.64/(126.56 + t/°C); \text{ temp range 60–176°C (Antoine eq., Dean 1985, 1992)} \]

\[ \log (P/kPa) = 5.9794 - 1256.783/(-133.487 + T/K); \text{ temp range 336–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log (P/kPa) = 6.10408 - 1322.62/(-126.87 + T/K); \text{ temp range 335–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log (P/mmHg) = -19.9205 - 4.3239 \times 10^3/(T/K) + 18.794 \cdot \log (T/K) - 5.0553 \times 10^{-2} \cdot (T/K) + 2.6161 \times 10^{-5} \cdot (T/K)^2; \text{ temp range 239–632 K (vapor pressure eq., Yaws 1994)} \]

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

1.909 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

1.880 (exptl., Hine & Mookerjee 1975)

2.656, 3.583 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.015 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988)

1.176 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

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

5.62 (gas stripping-GC, Shiu & Mackay 1997)

1.165 (wetted-wall column-GC, Altschuh et al. 1999)

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

2.53 (Hansch & Dunn III 1972)

2.41 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)

2.57 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

2.39 (RP-HPLC-k’ correlation, D’Ambroise & Hanai 1982)

2.60 (HPLC-k’ correlation, Funasaki et al. 1986)

2.65 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)

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

2.57 (generator column-GC, Schantz & Martire 1987)

2.57 (calculated-activity coeff. \( \gamma \), Schantz & Martire 1987)

1.83 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)

2.62 (recommended, Sangster 1989, 1993)

2.72 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

1.09 (calculated as per Mackay 1982, Schultz et al. 1990)

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

1.48 (calculated-MCI \( \chi \), Gerstl & Helling 1987)

1.14 (soil, quoted exptl., Meylan et al. 1992)

1.19 (soil, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)

1.14 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Volatilization: evaporation rate of \( 6.804 \times 10^{-6} \text{ mol cm}^{-2} \text{ h}^{-1} \) was determined by gravimetric method with an air flow rate of \( (50 \pm 1) \text{ L h}^{-1} \) at 20°C (Gückel et al. 1973).

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ as indicated. *Data at other temperatures see reference:

- Photooxidation $t_{1/2} = 0.24–2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical in air (Darnall et al. 1976)
- $k_{\text{OH}}(\text{exptl}) = (13.6 \pm 1.3) \times 10^{-12}$ cm$^{-1}$ molecule$^{-1}$ s$^{-1}$, $k_{\text{OH}}(\text{calc}) = 10.5 \times 10^{-12}$ cm$^{-1}$ molecule$^{-1}$ s$^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)
- $k_{\text{OH}}(\text{exptl}) = 1.36 \times 10^{-12}$ cm$^{-1}$ molecule$^{-1}$ s$^{-1}$, and $k_{\text{soln}} = 1.20 \times 10^{-11}$ cm$^{-1}$ molecule$^{-1}$ s$^{-1}$ for the reaction with OH radical in aqueous solution (Wallington et al. 1988b)
- $k_{\text{OH}} = (13.7 \pm 1.5) \times 10^{-12}$ cm$^{-3}$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (relative rate method, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

- Air: $t_{1/2} = 0.24–2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical in air (Darnall et al. 1976).

Surface water:

Sediment:

Soil:

Biota:

### TABLE 11.1.1.11.1
Reported aqueous solubilities of 1-heptanol at various temperatures

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FIGURE 11.1.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-heptanol.
TABLE 11.1.11.2
Reported vapor pressures of 1-heptanol at various temperatures and the coefficients for the vapor pressure equations

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

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\[\Delta H_v/(kJ \ mol^{-1}) = 68.66 \text{ at } 25°C\]

FIGURE 11.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1-heptanol.
11.1.1.12 1-Octanol (n-Octyl alcohol)

Common Name: 1-Octanol
Synonym: 1-octanol, n-octyl alcohol, capryl alcohol, heptylcarbinol
Chemical Name: n-octyl alcohol, 1-octanol
CAS Registry No: 111-87-5
Molecular Formula: C₈H₁₈O, CH₃(CH₂)₇OH
Molecular Weight: 130.228
Melting Point (°C):
   –14.8  (Lide 2003)
Boiling Point (°C):
   195.15  (Lide 2003)
Density (g/cm³ at 20°C):
   0.827  (Weast 1982–83)
   0.82499, 0.82157  (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
   158.0  (calculated-density, Rohrschneider 1973; Lande & Banerjee 1981)
   192.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hᶠus (kJ/mol):
   42.3  (Riddick et al. 1986)
Entropy of Fusion, ∆Sᶠus (J/mol K):
   56  (estimated, Yalkowsky & Valvani 1980)
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):
   586  (shake flask-interferometer, Butler et al. 1933)
   760  (30°C, shake flask-titration, Sobotka & Glick 1934.)
   420  (20°C, shake flask-surface tension, Addison 1945)
   590  (shake flask-turbidimeter, McBain & Richard 1946)
   500  (shake flask-titration, Crittenden & Hixon 1954)
   582  (estimated, McGowan 1954)
   490  (shake flask-surface tension, Kinoshita et al. 1958)
   495  (shake flask-turbidity, Shinoda et al. 1959)
   1000  (30°C, shake flask-turbidimeter, Rao et al. 1961)
   330  (calculated-Keq, Hansch et al. 1968)
   530  (15°C, shake flask-surface tension, Vochten & Petre 1973)
   600, 600  (40, 60°C, shake flask-titration, Lavrova & Lesteva 1976)
   10000, 5000  (95, 115°C, shake flask-polythermic method, Zhuravleva et al. 1977)
   540*  (recommended best value, IUPAC Solubility Data Series, temp range 15–115°C, Barton 1984)
   490*  (20.5°C, shake flask-GC/TC, measured range 20.5–90.3°C, Stephenson et al. 1984)
   517  (shake flask-GC, Li et al. 1992)
   417  (shake flask-GC, Li & Andren 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):
   11.06*  (25°C, extrapolated-modified isoteniscope data, measured range 60.12–110°C, Butler et al. 1935)
   log (P/mmHg) = 40.2105 – 4100/(T/K) – 10.35·log (T/K); temp range 20–110°C (isoteniscope measurements, Butler et al. 1935)
   18.8*  (extrapolated-regression of tabulated data, temp range 54–195.2°C, Stull 1947)
   log (P/mmHg) = 8.29442 – 2302.3/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
   7604*  (121.99°C, ebulliometry, measured range 121.99–195.28°C, Dreisbach & Shrader 1949)
5.28 (extrapolated-Antoine eq., ebulliometry- DTA, Kemme & Kreps 1969)
706.6* (78.9°C, ebulliometry-differential thermal analysis, measured range 78.9–195.3°C, Kemme & Kreps 1969)

\( \log (P/\text{mmHg}) = 6.62354 - \frac{1196.639}{124.107 + t/°C} \); temp range 78.9–195.3°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)


142* (54.88°C, comparative ebulliometry, measured range 328.03–386.96 K, data fitted to Chebyshev polynomial, Ambrose et al. 1974)

2.78 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

4.07, 32.3, 177 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)

\( \log (P/\text{mmHg}) = \left[ -0.2185 \times 14262.4/(T/K) \right] + 9.601156 \); temp range: 54–195°C, (Antoine eq., Weast 1972–73)

10.06, 6.89, 5.74, 9.95 (extrapolated-Antoine eq., Boublik et al. 1984)

\( \log (P/\text{Pa}) = 6.80512 - 1752.302/(174.07 + t/°C) \); temp range 54.88–113.9°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)

\( \log (P/\text{Pa}) = 5.98227 - 1322.952/(137.413 + t/°C) \); temp range 79.9–195.4°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

\( \log (P/\text{Pa}) = 5.87970 - 1260.554/(130.23 + t/°C) \); temp range 113.3–206.1°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

\( \log (P/\text{Pa}) = 6.00162 - 1356.232/(144.452 + t/°C) \); temp range 229.05–250.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

13.43 (calculated-Antoine eq., Dean 1985)

\( \log (P/\text{mmHg}) = 12.0701 - 4506.8/(319.9 + t/°C) \); temp range 0–80°C (Antoine eq., Dean 1985, 1992)

\( \log (P/\text{mmHg}) = 6.83790 - 1310.62/(136.05 + t/°C) \); temp range 70–195°C (Antoine eq., Dean 1985, 1992)

14.5 (static measurement, Berti et al. 1986)

10.0 (Riddick et al. 1986)

\( \log (P/\text{Pa}) = 5.88511 - 1264.322/(t/°C + 130.73) \); temp range not specified (Riddick et al. 1986)

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

\( \log (P/\text{Pa}) = 5.90052 - 1273.291/(–141.417 + T/K) \); temp range 386–480 K (Antoine eq.-I, Stephenson & Malanowski 1987)

\( \log (P/\text{Pa}) = 5.342 – 3343/(T/K); \) temp range 267–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)

\( \log (P/\text{Pa}) = 18.014 – 5507/(T/K); \) temp range 238–251 K (Antoine eq.-III, Stephenson & Malanowski 1987)

\( \log (P/\text{Pa}) = 5.7934 – 1208.201/(–149.366 + T/K); \) temp range 430–474 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

\( \log (P/\text{Pa}) = 6.39406 – 1540.599/(–114.618 + T/K); \) temp range 328–400 K (Antoine eq.-V, Stephenson & Malanowski 1987)

\( \log (P/\text{Pa}) = 5.90632 – 1276.86/(–140.996 + T/K); \) temp range 397–479 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

10.58 (Daubert & Danner 1989; quoted, Howard 1993)

\( \log (P/\text{mmHg}) = -26.3876 – 4.2263 \times 10^3/(T/K) + 21.093\log(T/K) - 5.0048 \times 10^{-2}\cdot(T/K) + 2.4611 \times 10^{-5}\cdot(T/K)^2; \) temp range 258–653 K (vapor pressure eq., Yaws 1994)

8.0* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)

\( \ln (P/\text{Pa}) = 13.058110 – 2443.493/(T/K – 162.071); \) temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

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

2.454 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

2.479 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

2.422 (exptl., Hine & Mookerjee 1975)

3.344, 6.085 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.537 (calculated-MCI \chi, Nirmalakhandan & Speece 1988)
Octanol/Water Partition Coefficient, log \(K_{OW}\):
- 3.15 (shake flask-CR, Collander 1951)
- 2.84 (calculated-\(\pi\) constant, Hansch et al. 1968)
- 3.03 (Hansch & Dunn III 1972)
- 2.95, 2.97; 2.84 (calculated-f const.; calculated-\(\pi\) constant, Rekker 1977)
- 2.97 (HPLC-k' correlation, Könemann et al. 1979)
- 2.80 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
- 2.92 (RP-HPLC-k' correlation, D'Amboise & Hanai 1982)
- 3.16 (shake flask-GC, Platford 1983)
- 2.97 (Hansch & Leo 1985)
- 3.27 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
- 2.14 (calculated-activity coeff. \(\gamma\) from UNIFAC, Banerjee 1988)
- 3.07 (recommended, Sangster 1989, 1993)
- 3.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{OA}\):
- 6.03 (calculated-measured \(\gamma^\infty\) in pure octanol and vapor pressure \(P\), Abraham et al. 2001)

Bioconcentration Factor, log BCF:
- 0.307 (calculated-\(K_{OW}\), Lyman et al. 1982; quoted, Howard 1993)
- 0.097 (calculated-\(S\), Lyman et al. 1982; quoted, Howard 1993)
- 1.65 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log \(K_{OC}\):
- 2.99 (soil, calculated-\(K_{OW}\), Lyman et al. 1982; quoted, Howard 1993)
- 2.14 (soil, calculated-\(S\), Lyman et al. 1982; quoted, Howard 1993)
- 1.56, 1.76 (quoted, calculated-MCI \(\chi\), Gerstl & Helling 1987)
- 1.56 (soil, quoted exp., Meylan et al. 1992)
- 1.45 (soil, calculated-MCI \(\chi\) and fragment contribution, Meylan et al. 1992)
- 1.56 (soil, calculated-MCI \(\chi\), Sabljic et al. 1995)

Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
- Volatilization: evaporation rate \(k = 1.752 \times 10^{-6}\) mol·cm\(^{-2}\)·h\(^{-1}\) was determined by gravimetric method with an air flow rate \(k = (50 \pm 1)\) L·h\(^{-1}\) at 20 ± 0.1°C (Gückel et al. 1973);
  - \(t_{1/2} \approx 1.8\) d from a model river of 1-m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry’s law constant (Lyman et al. 1982; quoted, Howard 1993);
  - \(t_{1/2} \approx 8.2\) d from a model pond with the consideration of adsorption (USEPA 1987; quoted, Howard 1993).
- 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 half-life of 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);
  - \(k \leq 0.8\) M\(^{-1}\) s\(^{-1}\) for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
  - \(k_{OH} = (13.6 \pm 1.3) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 298 K (Wallington et al. 1988a; Atkinson 1989)
  - \(k_{OH} = (14.4 \pm 1.5) \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 298 ± 2 K (relative rate method, Nelson et al. 1990)
  - \(k_{OH}(calc) = 11.67 \times 10^{-12}\) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) (molecular orbital calculations, Klamt 1996)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:
Half-Lives in the Environment:

Air: \( t_{\frac{1}{2}} = 0.24–2.4 \) h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); photooxidation \( t_{\frac{1}{2}} = 1.3 \) d in air, based on measured rate constant \( k = 1.195 \times 10^{-11} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) for the vapor-phase reaction with photochemically produced hydroxyl radical of \( 5 \times 10^5 \) cm\(^{-3}\) at 25°C in air (Atkinson 1987; quoted, Howard 1993).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:

**TABLE 11.1.1.12.1**

Reported aqueous solubilities of 1-octanol at various temperatures

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*“best” values

**FIGURE 11.1.1.12.1** Logarithm of mole fraction solubility \( \ln x \) versus reciprocal temperature for 1-octanol.
TABLE 11.1.1.12.2
Reported vapor pressures of 1-octanol at various temperatures and the coefficients for the vapor pressure equations

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

1. Butler et al. 1935

<table>
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<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>Stull 1947</th>
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bp/°C 194.5
D_{25} 0.8232

\begin{align*}
eq 4 & \quad P/mmHg \\
A & \quad 65.2106 \\
B & \quad 6190 \\
C & \quad 18.40
\end{align*}

\[ \Delta H_v/(kJ \text{ mol}^{-1}) = 72.93 \]

at 25°C

2. Ambrose & Sprake 1970

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**TABLE 11.1.12.2** (Continued)

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<th>t/°C</th>
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Antoine eq. for full range

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Data also fitted to Cragoe equation, see ref.

**FIGURE 11.1.12.2** Logarithm of vapor pressure versus reciprocal temperature for 1-octanol.
11.1.1.13 1-Nonanol

Common Name: 1-Nonanol
Synonym: n-nonyl alcohol
Chemical Name: 1-nonanol
CAS Registry No: 143-08-8
Molecular Formula: C9H20O, CH3(CH2)8OH
Molecular Weight: 144.254
Melting Point (°C):
–5 (Lide 2003)
Boiling Point (°C):
213.37 (Lide 2003)
Density (g/cm³ at 20°C):
0.8273 (Weast 1982–83)
Molar Volume (cm³/mol):
174.4 (20°C, Stephenson and Malanowski 1987)
214.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
Enthalpy of Sublimation, ∆Hsubl (kJ/mol):
Enthalpy of Fusion, ∆Hfus (kJ/mol):
Entropy of Fusion, ∆Sfus (J/mol K):
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):
140 (shake flask-surface tension, Kinoshita et al. 1958)
140 (15°C, shake flask-surface tension, Vochten and Petre 1973)
130 (recommended-IUPAC Solubility Data Series, Barton 1984)
280* (20°C, shake flask-GC/TC, measured range 9.8–90.5°C, Stephenson & Stuart 1986)
128 (20°C, shake flask/slow stirring-GC, Letinski et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (59.5°C, summary of literature data, temp range 59.5–213.5°C, Stull 1947)
746.6* (91.7°C, ebulliometry-differential thermal analysis, measured range 91.7–213.6°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.83667 – 1373.417/(133.968 + t°C); temp range 91.7–213.6°C, or pressure range 5.6–757.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
log (P/mmHg) = [-0.2185 × 14065.1/(T/K)] + 8.99150; temp range 69.5–231°C (Antoine eq., Weast 1972–73)
7.466 (20°C, extrapolated from data of Stull 1947, Gückel et al. 1973)
1.87 (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
12680* (152.15°C, ebulliometry, measured range 152–221.35°C, Hon et al. 1976)
0.106 (20°C, evaporation rate-gravimetric method, Gückel et al. 1982)
log (P/kPa) = 5.9049 – 1341.28/(-142.64 + T/K); temp range 381–495 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 5.9454 – 1366.566/(-139.73 + T/K); temp range 368–500 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 103.0308 –8.1526 × 10³/(T/K) –31.641-log(T/K) – 7.230 × 10⁻¹⁰·(T/K) + 6.0332 × 10⁻⁶·(T/K)²; temp range 280–690 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
1.675 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log \( K_{ow} \):  
- 3.77 (generator column-GC, Tewari et al. 1982)  
- 4.26 (shake flask, Log P Database, Hansch & Leo 1987)  
- 4.26 (recommended, Sangster 1993)  
- 4.26 (shake flask, 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 Constant, \( k \), and Half-Lives, \( t_\frac{1}{2} \):  

Half-Lives in the Environment:

### TABLE 11.1.1.13.1  
Reported aqueous solubilities of 1-nonanol at various temperatures  

**Stephenson & Stuart 1986**  

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<th>( t/\circ C )</th>
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**FIGURE 11.1.1.13.1**  
Logarithm of mole fraction solubility (ln \( x \)) versus reciprocal temperature for 1-nonanol.

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TABLE 11.1.13.2
Reported vapor pressures of 1-nonanol at various temperatures and the coefficients for the vapor pressure equations

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

(1) \hspace{1cm} (1a) \hspace{1cm} (2) \hspace{1cm} (2a) \hspace{1cm} (3) \hspace{1cm} (4)

Stull 1947
Kemme & Kreps 1969
Hon et al. 1976

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
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Antoine eq.  
\[ \text{eq. 2} \quad P/\text{mmHg} = A - B/T + C \log(T) \]

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1-Nonanol: vapor pressure vs. 1/T

FIGURE 11.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 1-nonanol.
11.1.1.14 1-Decanol

Common Name: 1-Decanol
Synonym: decyl alcohol
Chemical Name: 1-decanol
CAS Registry No: 112-30-1
Molecular Formula: C\textsubscript{10}H\textsubscript{22}O, CH\textsubscript{3}(CH\textsubscript{2})\textsubscript{8}CH\textsubscript{2}OH
Molecular Weight: 158.281
Melting Point (°C):
6.9 (Lide 2003)
Boiling Point (°C):
231.1 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.8297 (Weast 1982–83)
Molar Volume (cm\textsuperscript{3}/mol):
190.8 (20°C, calculated-density, Stephenson and Malanowski 1987)
236.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
50 (shake flask-turbidimetric method, Stearns et al. 1947)
36 (20°C, shake flask-surface tension, Addison and Hutchinson 1949)
50 (shake flask-turbidimetric method-photometer, Harkins and Oppenheimer 1949)
37 (shake flask-surface tension, Kinoshita et al. 1958)
32 (15°C, shake flask-surface tension, Vochten and Petre 1973)
10000, 8000 (102.5, 120.5°C, polythermic method, Zhuravleva et al. 1977)
37* (recommended-IUPAC Solubility Data Series, temp range 15–120°C, Barton 1984)
210* (29.6°C, shake flask-GC/TC, measured range 29.6–90.4°C, Stephenson 1992)
35.9 (dialysis tubing equilibration-GC, Etzweiler 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):
133.3* (69.5°C, summary of literature data, temp range 69.5–231.0°C, Stull 1947)
747* (105.0°C, ebulliometry-differential thermal analysis, measured range 105–231°C, Kemme & Kreps 1969)
log (P/mmHg) = 6.39379 – 1180.306/(104.321 + t/°C); temp range 105–231°C, or pressure range 5.6–757.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
1.0* (comparative ebulliometry, measured range 127.261–255.2°C, Ambrose & Sprake 1970)
log (P/Pa) = 5.86571 – 1373.916/(T/K – 147.202); temp range 127.16–255.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
124* (76.23°C, comparative ebulliometry, measured range 349.38–406.19 K, data fitted to Chebyshev polynomial, Ambrose et al. 1974)
log (P/mmHg) = [–0.2185 × 13849.2/(T/K)] + 9.115470; temp range 59.5–213.5°C (Antoine eq., Weast 1972–73)
0.5866 (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
1.10 (20°C, evaporation rate-gravimetric method, Gückel 1982)
log (P/kPa) = 5.76028 – 1315.079/(119.128 + t/°C), temp range 105–231°C (Antoine eq. derived from exptl. data of Kemme & Kreps 1969, Boublík et al. 1984)

log (P/kPa) = 5.84611 – 1365.892/(124.619 + t/°C), temp range 127.2–255.2°C (Antoine eq. derived from data of Ambrose & Sprake 1970, Boublík et al. 1984)

log (P/kPa) = 17.615 – 6028/(T/K); temp range 264–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.57397 – 1761.308/(–113.992 + T/K); temp range 349–410 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 5.8587 – 1374.347/(-147.547 + T/K); temp range 405–528 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 111.7949 –8.3502 × 10^3/(T/K) –34.786·log(T/K) + 3.3682 × 10–10·(T/K) + 7.2697 × 10–6·(T/K)^2; temp range 268–673 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
- 2.689 (computer value, Yaws et al. 1991)
- 3.222 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
- 3.98 (HPLC-RT correlation, D’Amboise & Hani 1982)
- 4.57 (shake flask, Log P Database, Hansch & Leo 1987)
- 4.57 (recommended, Sangster 1993)

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

Bioconcentration Factor, log BCF or log K_{B}:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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<th>TABLE 11.1.1.14.1</th>
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mp/°C | 5
Alcohols

FIGURE 11.1.14.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-decanol.

TABLE 11.1.14.2
Reported vapor pressures of 1-decanol at various temperatures and the coefficients for the vapor pressure equations

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Stull 1947

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Kemme & Kreps 1969

differential thermal analysis

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Ambrose & Sprake 1970

comparative ebulliometry

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Ambrose & Sprake 1974

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| Antoine eq |
| eq. 2 | P/mmHg |
| A | 6.39397 |

summary of literature data

differential thermal analysis

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**FIGURE 11.1.1.14.2** Logarithm of vapor pressure versus reciprocal temperature for 1-decanol.
11.1.1.15 Ethylene glycol

Common Name: Ethylene glycol
Synonym: 1,2-ethanediol, 1,2-dihydroxyethane, MEG
Chemical Name: 1,2-ethanediol, ethylene glycol
CAS Registry No: 107-21-1
Molecular Formula: C₂H₆O₂, HOCH₂CH₂OH
Molecular Weight: 62.068
Melting Point (°C): –12.69 (Lide 2003)
Boiling Point (°C): 197.3 (Lide 2003)
Density (g/cm³ at 20°C): 1.1088 (Weast 1982–83)
Molar Volume (cm³/mol):
55.8 (Rohrschneider 1973)
66.6 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
14.22 (Dean 1985)
14.24 (Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₚ (kJ/mol):
9.958 (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):
miscible (Dean 1985; Howard 1990; Yaws et al. 1990)
miscible (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):
22.39 (extrapolated-Antoine eq., differential manometer, Gallaugher & Hibbert 1937)
log (P/mmHg) = 9.2087 – 2976.6/(T/K); temp range 40–120°C (Antoine eq. from differential Hg manometry measurements, Gallaugher & Hibbert 1937)
133.3* (53.0°C, summary of literature data, temp range 53.0–197.3°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 14032.4/(T/K)] + 9.394685; temp range: 53–197.3°C (Antoine eq., Weast 1972–73)
11.70* (ebulliometry, extrapolated-Antoine eq., measured range 270–310 K, Ambrose & Hall 1981)
log (P/kPa) = 11.1828 – 2611.2/[(T/K) – 40.0]; temp range 270–310 K (ebulliometry, Antoine eq., Ambrose & Hall 1981)
log (P/kPa) = 6.83995 – 1818.591/[(T/K) – 94.499]; temp range 374.01–495.4 K (Antoine eq., ebulliometry, Ambrose & Hall 1981)
log (P/mmHg) = 23.7259 – 4648.55/(T/K) – 503391/(T/K)²; temp range 283–373 K (empirical vapor pressure eq., gas saturation, Hales et al. 1981)
14.90 (20°C, evaporation method, Gückel et al. 1982)
0.73, 9.30 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.69339 – 1093.154/(98.821 + t/°C); temp range 122.5–186.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 7.13856 – 2035.185/(936.936 + t/°C); temp range 50–200°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
11.86 (extrapolated-Antoine eq., Dean 1985)
11.7 (Riddick et al. 1986)
log \left( \frac{P}{kPa} \right) = 6.83995 - 1818.591/(178.651 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log \left( \frac{P}{kPa} \right) = 8.3726 - 2994.4/(T/K), temp range 130–190°C, (Antoine eq., Riddick et al. 1986)

log \left( \frac{P}{mmHg} \right) = 8.0908 - 2088.9/(203.5 + t/°C); temp range 50–200°C (Antoine eq., Dean 1985, 1992)

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

log \left( \frac{P}{kPa} \right) = 8.69612 - 1817.439/(–95.859 + T/K); temp range 363–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \left( \frac{P}{mmHg} \right) = 82.4062 - 6.3472 \times 10^3/(T/K) - 25.433 \cdot \log(T/K) - 2.3732 \times 10^{-9} \cdot (T/K) + 8.7467 \times 10^{-6} \cdot (T/K)^2; temp range 160–645 K (vapor pressure eq., Yaws 1994)

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

0.006 (calculated-C W/CA, Hine & Mookerjee 1975)
5.81 \times 10^{-6}, 2.37 \times 10^{-5} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

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

–1.93 (shake flask, Hansch & Leo 1979)
–1.34 (shake flask-RC, Cornford 1982)
–1.36 (shake flask, Log P Database, Hansch & Leo 1987)
–1.36 (recommended, Sangster 1993)
–1.36 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

1.00 (golden ide, after 3 d, Freitag et al. 1985)
2.28 (algae, after 1 d, Freitag et al. 1985)
2.30 (activated sludge, after 5 d, Freitag et al. 1985)

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

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

Volatilization: evaporation rate \( k = 2.915 \times 10^{-6} \) mol cm\(^{-2}\) h\(^{-1}\) was determined by gravimetric method with an air flow rate \( k = (50 \pm 1) \) L h\(^{-1}\) at 20 ± 0.1°C (Gückel et al. 1973); evaporation rate \( k = 2.97 \times 10^{-8} \) mol cm\(^{-2}\) h\(^{-1}\) was determined at 20°C (Gückel et al. 1982).

Photolysis:

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

photoxidation \( t_{1/2} = 267\) d-64.6 yr in water, based on measured rate constant for the reaction with OH radical (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

photoxidation \( t_{1/2} = 0.24–2.4 \) h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

\( k_{OH} = (7.7 \pm 1.1) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 295 K in air (Wiedermann & Zetzsch 1982; quoted, Atkinson 1985)

photoxidation \( t_{1/2} = 8.3–83 \) h in air, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

Hydrolysis:

Biodegradation:

\( k = 41.7 \) mg COD g\(^{-1}\) h\(^{-1}\), average rate based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); \( k = 0.026–0.035 \) h\(^{-1}\) in 30 mg/L activated sludge after a time lag of 10–15 h (Urano & Kato 1986b)

\( t_{aq. aerobic} = 48–288 \) h, based on grab sample from river die-away studies (Evans & David 1974; selected, Howard et al. 1991);
Alcohols 2555

\[ t_{1/2}(\text{aq. anaerobic}) = 192–1152 \text{ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).} \]

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

Half-Lives in the Environment:
Air: \( t_{1/2} = 0.24–2.4 \text{ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);} \)
photooxidation \( t_{1/2} = 8.3–83 \text{ h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);} \)
atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).
Surface water: photooxidation \( t_{1/2} = 267 \text{ d-64.6 yr, based on measured rate constant for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991);} \)
\( t_{1/2} = 48–288 \text{ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).} \)
Groundwater: \( t_{1/2} = 96–576 \text{ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).} \)
Sediment:
Soil: \( t_{1/2} = 48–288 \text{ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).} \)
Biota

### TABLE 11.1.1.15.1
Reported vapor pressures of ethylene glycol at various temperatures and the coefficients for the vapor pressure equations

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

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FIGURE 11.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for ethylene glycol.
11.1.1.16 Allyl alcohol

Common Name: Allyl alcohol

Synonym: propenyl alcohol, 2-propen-1-ol, 1-propene-3-ol, vinylcarbinol

Chemical Name: allyl alcohol, 1-propene-3-ol, 2-propen-1-ol

CAS Registry No: 107-18-6

Molecular Formula: C₃H₆O, CH₂=CHCH₂OH

Molecular Weight: 58.079

Melting Point (°C):
-129 (Stull 1947; Weast 1982–83; Verschueren 1983; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):
97.1 (Weast 1982–83; Dean 1985; Riddick et al. 1986)
97 (Lide 2003)

Density (g/cm³ at 20°C):
0.854 (Weast 1982–83; Dean 1985)
0.85511 (15°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
64.8 (Kamlet et al. 1986; Leahy 1986)
74.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pKₐ:
15.5 (Riddick et al. 1986)

Enthalpy of Fusion, ΔHₘ₀ (kJ/mol):

Entropy of Fusion, ΔSₘ₀ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS = 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)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2666* (21.7°C, temp range –20 to 96.6°C, Stull 1947)
3140 (Hoy 1970)

log (P/mmHg) = [–0.2185 × 10577.7/(T/K)] + 9.143231; temp range –20 to 96.6°C (Antoine eq., Weast 1972–73)
2666, 4266 (20°C, 30°C, Verschueren 1983)
3750 (Riddick et al. 1986)

log (P/kPa) = 31.75070 – 3451.8/(–38.295 + T/K); temp range 253–370 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.506 (calculated-Cₙ/Cₜ, Hine & Mookerjee 1975)
0.510 (calculated-bond contribution, Hine & Mookerjee 1975)
0.564 (computed, Hine & Mookerjee 1975)
Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 0.17 (shake flask, Hansch & Leo 1979)
- 0.17 (recommended, Sangster 1989)
- 0.17 (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:

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:
- photooxidation \( t_\text{1/2} = 334 \text{ d-37 yr} \), based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991)
- photooxidation \( t_\text{1/2} = 2.2–22 \text{ h} \), based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

\[ k_{OH} = 25.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 440 \text{ K} \]  
(Atkinson 1989)

Biodegradation: \( t_\text{1/2(aq. aerobic)} = 24–168 \text{ h} \), based on estimated unacclimated aqueous aerobic biodegradation screening test data (Sasaki 1978; quoted, Howard et al. 1991); \( t_\text{1/2(aq. anaerobic)} = 96–672 \text{ h} \), 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 \( t_\text{1/2} = 2.2–22 \text{ h} \), based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation \( t_\text{1/2} = 334 \text{ d-37 yr} \), based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991).

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

Sediment:

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

Biota:

**TABLE 11.1.16.1**
Reported vapor pressures of allyl alcohol at various temperatures

<table>
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<th>Stull 1947 summary of literature data</th>
<th>Lubomska &amp; Malanowski 2004 ebulliometry</th>
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#### FIGURE 11.1.1.16.1

Logarithm of vapor pressure versus reciprocal temperature for allyl alcohol.

Allyl alcohol: vapor pressure vs. 1/T

- **Lubomska & Malanowski 2004**
- **Stull 1947**

b.p. = 97 °C
11.1.1.17  Cyclohexanol

Common Name: Cyclohexanol
Synonym: adronol, anal, cyclohexylalcohol, hexahydropbenol, hexalin, hydralin, hydrophenol
Chemical Name: cyclohexanol
CAS Registry No: 108-93-0
Molecular Formula: C₆H₁₁OH
Molecular Weight: 100.158
Melting Point (°C): 25.93 (Lide 2003)
Boiling Point (°C): 160.84 (Lide 2003)
Density (g/cm³): 0.9624 (Lide 2003)
Molar Volume (cm³/mol):
104.0  (calculated-density, Lande & Banerjee 1981)
125.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol): 1.70 (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 or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
37000*  (shake flask-synthetic method, temp range 7.2–184.72°C, Sidgwick & Sutton 1930)
39200  (shake flask-interferometry, Hansen et al. 1949)
32920  (residue volume, Booth & Everson 1942)
40000*  (20°C, synthetic method, measured range 0–184°C, Zil’berman 1951)
48960  (shake flask-interferometry, Donahue & Bartell 1952)
36000  (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
38000*  (recommended “best” value, IUPAC Solubility Data Series, temp range 0–180°C, Baron 1984)
37500  (selected, Riddick et al. 1986)
44400*  (19.7°C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson & Stuart 1986)
38200  (selected, Yaws et al. 1990)
37500  (dialysis tubing equilibration-GC. Etzweiler 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):
467*  (34.0°C, Ramsay-Young method, measured range 34.0–149.0°C, Gardner & Brewer 1937)
133.1*, 194  (21°C, interpolated-regression of tabulated data, temp range 21–161°C, Stull 1947)
7177*  (93.73°C, temp range 93.73–160.70°C, Novak et al. 1960; quoted, Boublik et al. 1984)
log (P/mmHg) = [–0.218 × 11935.8/(T/K)] + 8.909086; temp range 21–161°C (Antoine eq., Weast 1972–73)
174.8  (calculated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 434.658/(T/K)] × 10^8{0.951396 – 8.46102 × 10⁻¹(T/K) + 8.87926 × 10⁻²(T/K)^2}; temp range 294.15–434.15 K (Cox eq., Chao et al. 1983)
37.53  (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 6.2553 – 912.87/(109.13 + t/°C); temp range 94–161°C (Antoine eq., Dean 1985, 1992)
1300  (56°C, Riddick et al. 1986)
log (P/kPa) = 5.92859 – 1199.10/(t/°C + 145.0); temp range 107–160°C (Riddick et al. 1986)
97.36  (interpolated, solid, Antoine eq.-I, Stephenson & Malanowski 1987)
Alcohols

80.0, 84.85 (extrapolated, liquid, Antoine eq.-I and II, Stephenson & Malanowski 1987)
\[
\log (P_1/kPa) = 9.631 - 3173.1/(T/K); \text{ temp range 272–298 K (Antoine eq.-I, for solid, Stephenson & Malanowski 1987)}
\]
\[
\log (P_2/kPa) = 6.1634 - 1318.5/(–116.55 + T/K); \text{ temp range 318–434 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)}
\]
\[
\log (P_3/kPa) = 6.27792 - 1381.8/(–110.132 + T/K); \text{ temp range 300–434 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)}
\]
106.6 (Daubert & Danner 1989)
14.66, 196.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)
\[
\log (P/mmHg) = 49.9123 - 4.8446 \times 10^3/(T/K) - 13.711 \cdot \log(T/K) + 3.5451 \times 10^{-9}\cdot(T/K) + 1.5932 \times 10^{-6}\cdot(T/K)^2;
\text{ temp range 297–625 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa·m³/mol):
0.581 (calculated C sub W/P, Hine & Mookerjee 1975)
2.48, 2.37 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
0.281 (calculated-P/C, Howard 1993)
0.278 (correlated-molecular structure, Russell et al. 1992)
0.446 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K OW:
1.23 (shake flask-AS, Hansch & Anderson 1967, Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
1.36 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)
1.23 (recommended, Sangster 1989, 1993)
1.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K OA:
5.18 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.708 (estimated-K OW, Lyman et al. 1990)
0.176 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, log K OC:
2.045 (soil, estimated-K OW, Lyman et al. 1990; quoted, Howard 1993)
1.114 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization: t½ ~145 d estimated from a model environmental pond with the consideration of the effect of adsorption (USEPA 1987; quoted, Howard 1993);
based on the Henry’s law constant, t½ ~13.3 d from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s at 25°C (Lyman et al. 1990; quoted, Howard 1993).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k OH for reaction with OH radical, k NO3 with NO3 radical and k O3 with O3 or as indicated, *data at other temperatures see reference:
k OH = 17.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with OH radical concentration of } 5 \times 10^8 \text{ per cm}^3 \text{ in air at 25°C corresponds to an atmosphere t½ = 22 h (Atkinson 1987; quoted, Howard 1993)}
Hydrolysis:
Biodegradation: average rate of biodegradation k = 28.0 mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).
Biotransformation:
Bioconcentration Uptake (k1) and Elimination (k2) Rate Constants:
Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 22$ h, based on estimated reaction rate constant of $17.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the vapor phase reaction with $5 \times 10^5$ hydroxyl radical per cm$^3$ in air at 25°C (Howard 1993).

Surface water:
Ground water:
Sediment:
Soil:
Biota:

### TABLE 11.1.17.1
Reported aqueous solubilities of cyclohexanol at various temperatures

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Zh. Fis. Khim. 24, 776–8
FIGURE 11.1.1.17.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohexanol.

TABLE 11.1.1.17.2
Reported vapor pressures of cyclohexanol at various temperatures and the coefficients for the vapor pressure equations

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

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in Boublik et al. 1984

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Gardner & Brewer 1937
Stull 1947
Novak et al. 1960

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FIGURE 11.1.17.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanol.
11.1.1.18  Benzyl alcohol

Common Name: Benzyl alcohol
Synonym: benzenemethanol, (hydroxymethyl)benzene, o-hydroxy toluene, phenylcarbinol, phenylmethanol
Chemical Name: benzyl alcohol
CAS Registry No: 100-51-6
Molecular Formula: C7H8O, C6H5CH2OH
Molecular Weight: 108.138
Melting Point (°C):
  –15.4  (Lide 2003)
Boiling Point (°C):
  205.31  (Lide 2003)
Density (g/cm³ at 20°C):
  1.04555, 1.04156  (20°C, 25°C, Dreisbach 1955)
  1.04127  (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  103.5  (calculated-density, Rohrschneider 1973)
  125.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
  48.13, 61.42  (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
  17.406  (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):
  38020  (Seidell 1941)
  34200  (estimated, McGowan 1954)
  38000  (20–25°C, shake flask-GC, Urano et al. 1982)
  35000  (20°C, Verschueren 1983)
  42900  (shake flask-LSC, Banerjee 1985)
  43000*  (20.1°C, shake flask-GC/TC, measured range 0–50°C, Stephenson & Stuart 1986)
  46070  (shake flask-GC, Li et al. 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*  (60.9°C, static method, measured range 60.9–152.1°C, Kahlbaum 1898)
  26.7*  (38.8°C, ebulliometry, measured range 38.8–151.6°C, Gardner & Brewer 1937)
  15.40*  (extrapolated-regression of tabulated data, temp range 58–205.7°C, Stull 1947)
log (P/mmHg) = 7.90550 – 2187.8/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
  6287*  (122.52°C, ebulliometry, measured range 122.52–205.41°C, Dreisbach & Shrader 1949)
  19.59  (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.58200 – 1904.3/(200.0 + t/°C); temp range 112–330°C (Antoine eq. for liquid state, Dreisbach 1955)
  12.0  (Hoy 1970)
log (P/mmHg) = [–0.2185 × 14093.2/(T/K)] + 9.391874; temp range 58–204.7°C (Antoine eq., Weast 1972–73)
log (P/Pa) = 29.0 – 7958/(T/K); temp range 29.5–60.1°C (Antoine eq., gas saturation, Grayson & Fosbraey 1982)
  4.750  (extrapolated-Cox eq., Chao et al. 1983)
log \( P/\text{mmHg} = \left[ 1 - 479.624/(T/K) \right] \times 10^4 \left[ \frac{1.02742 - 6.26739 \times 10^{-4} \cdot (T/K) + 1.28791 \times 10^{-7} \cdot (T/K)^2}{(T/K)} \right] ; \) temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)

12.07, 9.69 (extrapolated-Antoine eq., Boublík et al. 1984)

log \( P/\text{Pa} = 6.34897 - 1650.313/(174.623 + t/°C) \); temp range 122.5–205.4°C (Antoine eq. from reported exper. data of Dreisbach & Shrader 1949, Boublík et al. 1984)

log \( P/\text{Pa} = 6.39383 - 1655.003/(171.85 + t/°C) \); temp range 38.8–151.6°C (Antoine eq. from reported exper. data, Boublik et al. 1984)

11.72 (extrapolated-Antoine eq., Dean 1985)

log \( P/\text{Pa} = 7.19817 - 1632.593/(172.79 + t/°C) \); temp range 122–205°C (Antoine eq., Dean 1985, 1992)

15.0 (selected, Riddick et al. 1986)

log \( P/\text{Pa} = 8.963 - 3214/(T/K) \); temp range not specified (Antoine eq., Riddick et al. 1986)

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

log \( P/\text{Pa} = 6.7069 - 1904.3/(–73.15 + T/K) \); temp range 385–573 K (Antoine eq-I., Stephenson & Malanowski 1987)

7.395 (ebulliometry, fitted to Antoine eq., Ambrose & Ghiassiee 1990)

12.0 (calculated-Wagner eq., Ambrose & Ghiassiee 1990)

log \( P/\text{mmHg} = –36.2189 – 3.3475 \times 10^3/(T/K) + 23.337 \cdot \log(T/K) – 4.46 \times 10^{-2} \cdot (T/K) + 2.1443 \times 10^{-5} \cdot (T/K)^2 \); temp range 258–677 K (vapor pressure eq., Yaws 1994)

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

0.0231 (quoted estimated value of Hine & Mookerjee 1975, Howard 1993)

0.0396 (calculated-P/C, Howard 1993)

< 0.0273 (wetted-wall column-GC, Altschuh et al. 1999)

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

1.10 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968)

1.10 ± 0.02 (shake flask-UV, Iwasa et al. 1965)

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

1.10 (shake flask-RC, Cornford 1982)

1.00 (shake flask-UV, Mayer et al. 1982)

1.16 ± 0.02 (exptl.-ALPM, Garst & Wilson 1984)

1.06 (HPLC-k’ correlation, Eadsforth 1986)

1.58 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)

1.05 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

1.05 (recommended, Sangster 1989, 1993)

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

0.96 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)

1.10 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log \( BCF \):

0.602 (calculated-\( K_{ow} \), Lyman et al. 1982; quoted, Howard 1993)

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

1.193 (red-brown Australian soil with 1.09% organic carbon, Briggs 1981; quoted, Howard 1993)

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

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

Volatilization: estimated \( t_{1/2} = 97 \) d for a model river of 1 m deep, flowing at 1 m/s with wind velocity of 3 m/s (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, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures see reference:
Alcohols

\[ k_{\text{OH}} = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1989)} \]

\[ k_{\text{OH}}(\text{calc}) = 7.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \text{ estimated from Atmospheric Oxidation Program; } k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \text{ and } k_{\text{OH}}(\text{calc}) = 7.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ estimated from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)} \]

\[ k_{\text{OH}}(\text{calc}) - 0.85 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (SAR structure-activity relationship, Kwok & Atkinson 1995)} \]

Hydrolysis:

Biodegradation: biodegradation rate constant \( k = 0.042–0.062 \text{ h}^{-1} \text{ in } 30 \text{ mg L}^{-1} \text{ activated sludge after a lag time of } 5–15 \text{ h (Urano & Kato 1986).} \]

Biotransformation:

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

Half-Lives in the Environment:

- **Air:** the estimated \( t_\text{d} \approx 2 \text{ d} \) for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1993).

- **Surface water:**
- **Groundwater:**
- **Sediment:**
- **Soil:**
- **Biota:**

### TABLE 11.1.1.18.1

Reported aqueous solubilities of benzyl alcohol at various temperatures

**Stephenson & Stuart 1986**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( S/\text{g·m}^{-3} )</th>
</tr>
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<tr>
<td>0</td>
<td>48000</td>
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<td>9.8</td>
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<td>45000</td>
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<td>50.0</td>
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**FIGURE 11.1.1.18.1** Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for benzyl alcohol.
### TABLE 11.1.18.2
Reported vapor pressures of benzyl alcohol at various temperatures and the coefficients for the vapor pressure equations

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

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<tr>
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<th></th>
</tr>
</thead>
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<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>60.9</td>
<td>133.3</td>
<td>38.8</td>
<td>26.7</td>
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<tr>
<td>67.8</td>
<td>266.6</td>
<td>42.5</td>
<td>80.0</td>
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<td>72.9</td>
<td>400.0</td>
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<td>106.7</td>
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<td>77.2</td>
<td>533.3</td>
<td>50.5</td>
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<td>80.8</td>
<td>666.6</td>
<td>85.2</td>
<td>906.6</td>
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<td>92.8</td>
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<td>97.2</td>
<td>1747</td>
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<td>105.3</td>
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<td>3333.06</td>
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<td>113.4</td>
<td>3999.7</td>
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<td>101325</td>
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<td>116.7</td>
<td>4666.3</td>
<td>mp/°C</td>
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<td>5332.9</td>
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<td>124.4</td>
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<td>9999.2</td>
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<td>141.3</td>
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</tr>
<tr>
<td>152.1</td>
<td>19998</td>
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</table>

**Dreisbach & Shrader 1949 (ebulliometry)**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
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<tbody>
<tr>
<td>122.52</td>
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<td>127.12</td>
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<td>130.90</td>
<td>8851</td>
</tr>
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<td>134.28</td>
<td>10114</td>
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<td>147.09</td>
<td>16500</td>
</tr>
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<td>190.50</td>
<td>67661</td>
</tr>
<tr>
<td>205.41</td>
<td>101325</td>
</tr>
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</table>
**FIGURE 11.1.18.2** Logarithm of vapor pressure versus reciprocal temperature for benzyl alcohol.
### 11.2 SUMMARY TABLES AND QSPR PLOTS

#### TABLE 11.2.1
Summary of physical properties of alcohols

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C</th>
<th>Molar volume, V_m cm^3/mol</th>
<th>MW/ρ at 20°C</th>
<th>Le Bas</th>
</tr>
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<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>CH_3OH</td>
<td>32.042</td>
<td>−97.53</td>
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<td>40.49</td>
<td>37.0</td>
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<tr>
<td>Ethanol</td>
<td>64-17-5</td>
<td>C_2H_5OH</td>
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<td>−114.14</td>
<td>78.29</td>
<td>1</td>
<td>58.36</td>
<td>59.2</td>
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<tr>
<td>Propanol (n-Propyl alcohol)</td>
<td>71-23-8</td>
<td>C_3H_7OH</td>
<td>60.095</td>
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<td>97.2</td>
<td>1</td>
<td>74.79</td>
<td>81.4</td>
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<tr>
<td>Isopropanol (i-Propyl alcohol)</td>
<td>67-63-0</td>
<td>iC_3H_7OH</td>
<td>60.095</td>
<td>−87.9</td>
<td>82.3</td>
<td>1</td>
<td>76.51</td>
<td>81.4</td>
<td></td>
</tr>
<tr>
<td>1-Butanol (n-Butyl alcohol)</td>
<td>71-36-3</td>
<td>C_4H_9OH</td>
<td>74.121</td>
<td>−88.6</td>
<td>117.73</td>
<td>1</td>
<td>91.56</td>
<td>103.6</td>
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<td>Isobutanol (i-Butyl alcohol)</td>
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<td>iC_4H_9OH</td>
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<td>107.89</td>
<td>1</td>
<td>92.47</td>
<td>103.6</td>
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<td>sec-Butyl alcohol</td>
<td>78-92-2</td>
<td>xC_4H_9OH</td>
<td>74.121</td>
<td>−88.5</td>
<td>99.51</td>
<td>1</td>
<td>91.90</td>
<td>103.6</td>
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<td>tert-Butyl alcohol</td>
<td>75-65-0</td>
<td>tC_4H_9OH</td>
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<td>25.69</td>
<td>82.4</td>
<td>1</td>
<td>94.88</td>
<td>103.6</td>
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<tr>
<td>1-Pentanol (n-Amyl alcohol)</td>
<td>71-41-0</td>
<td>C_5H_11OH</td>
<td>88.148</td>
<td>−77.6</td>
<td>137.98</td>
<td>1</td>
<td>108.23</td>
<td>125.8</td>
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<tr>
<td>2-Pentanol</td>
<td>6032-29-7</td>
<td>C_5H_11OH</td>
<td>88.148</td>
<td>−73</td>
<td>119.3</td>
<td>1</td>
<td>108.91</td>
<td>125.8</td>
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<tr>
<td>1-Hexanol</td>
<td>111-27-3</td>
<td>C_6H_13OH</td>
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<td>−47.4</td>
<td>157.6</td>
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<td>124.79</td>
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<td>1-Heptanol</td>
<td>111-70-6</td>
<td>C_7H_15OH</td>
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<td>176.45</td>
<td>1</td>
<td>141.38</td>
<td>170.2</td>
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<tr>
<td>1-Octanol (n-Octyl alcohol)</td>
<td>111-87-5</td>
<td>C_8H_17OH</td>
<td>130.228</td>
<td>−14.8</td>
<td>195.16</td>
<td>1</td>
<td>157.85</td>
<td>192.4</td>
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<td>1-Nonanol</td>
<td>143-08-8</td>
<td>C_9H_19OH</td>
<td>144.254</td>
<td>−5</td>
<td>213.37</td>
<td>1</td>
<td>174.37</td>
<td>214.6</td>
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<tr>
<td>1-Decanol</td>
<td>112-30-1</td>
<td>C_{10}H_{21}OH</td>
<td>158.281</td>
<td>6.9</td>
<td>231.1</td>
<td>1</td>
<td>190.77</td>
<td>236.8</td>
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<tr>
<td>Ethylene glycol</td>
<td>107-21-1</td>
<td>(CH_{2}OH)_2</td>
<td>62.068</td>
<td>−12.69</td>
<td>197.3</td>
<td>1</td>
<td>55.98</td>
<td>66.6</td>
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<td>107-18-6</td>
<td>C_2H_5OH</td>
<td>58.079</td>
<td>−129</td>
<td>97</td>
<td>1</td>
<td>67.92</td>
<td>74.0</td>
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<td>96-41-3</td>
<td>C_5H_10OH</td>
<td>86.132</td>
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<td>106.9</td>
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<tr>
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<td>108-93-0</td>
<td>C_6H_{11}OH</td>
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<td>25.93</td>
<td>160.84</td>
<td>1</td>
<td>104.07</td>
<td>125.6</td>
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<td>Benzyl alcohol</td>
<td>100-51-6</td>
<td>C_7H_15OH</td>
<td>108.138</td>
<td>−15.4</td>
<td>205.31</td>
<td>1</td>
<td>103.85</td>
<td>125.6</td>
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### TABLE 11.2.2
Summary of selected physical-chemical properties of alcohols at 25°C

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<tr>
<th>Compound</th>
<th>Solubility</th>
<th>Henry's law constant H/(Pa·m³/mol)</th>
<th>( \log K_{ow} )</th>
<th>( \text{calc} ) P/C</th>
<th>( \text{exptl} ) (a)</th>
<th>( \text{exptl} ) (b)</th>
<th>( \text{exptl} ) (c)</th>
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<tr>
<td>Methanol</td>
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<td></td>
<td>16210</td>
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<td>0.45</td>
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<tr>
<td>Ethanol</td>
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<td></td>
<td>7800</td>
<td>0.31</td>
<td>0.53</td>
<td>0.527</td>
</tr>
<tr>
<td>Propanol</td>
<td>miscible</td>
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<td></td>
<td>2780</td>
<td>0.25</td>
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<td>0.751</td>
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<tr>
<td>Isopropanol</td>
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<td></td>
<td>5700</td>
<td>0.05</td>
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<td>900</td>
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<td>( \text{sec}-\text{Butyl alcohol} )</td>
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<td>( \text{tert}-\text{Butyl alcohol} )</td>
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<td>1.23</td>
<td>0.224</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzy alcohol</td>
<td>80</td>
<td>0.7398</td>
<td>12</td>
<td>1.10</td>
<td>16.22</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(a) Butler et al. 1935  
(b) Buttery et al. 1969  
(c) Snider & Dawson 1985
### TABLE 11.2.3
Suggested half-life classes of alcohols in various environmental compartments at 25°C

<table>
<thead>
<tr>
<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Ethanol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Propanol (n-Propyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Isopropanol (i-Propyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>1-Butanol (n-Butyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Isobutanol (i-Butyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>tert-Butyl alcohol</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>1-Pentanol (n-Amyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>1-Hexanol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>1-Octanol (n-Octyl alcohol)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Ethylene glycol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Allyl alcohol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Cyclohexanol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Benzyl alcohol</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
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</table>

where,

<table>
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<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>1,000–5,000</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>~ 5 years</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>

**FIGURE 11.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.
FIGURE 11.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.

FIGURE 11.2.3 Octanol-water partition coefficient versus Le Bas molar volume for alcohols.
FIGURE 11.2.4 Henry's law constant versus Le Bas molar volume for alcohols.

FIGURE 11.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alcohols.
11.3 REFERENCES


De Santis, R., Marrelli, L., Muscetta, P.N. (1976) Liquid-liquid equilibria in water-aliphatic alcohol systems in the presence of sodium


# 12 Aldehydes and Ketones

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<th>Page</th>
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<td>12.1.1.4 Butanal (n-Butyraldehyde)</td>
<td>2600</td>
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<tr>
<td>12.1.1.5 2-Propenal (Acrolein)</td>
<td>2605</td>
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<td>2609</td>
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<td>2613</td>
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<td>12.1.2.1 Acetone</td>
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<td>12.1.2.5 Methyl isobutyl ketone (MIBK)</td>
<td>2644</td>
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<tr>
<td>12.1.2.6 2-Hexanone (Methyl butyl ketone)</td>
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<tr>
<td>12.1.2.7 2-Heptanone</td>
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<tr>
<td>12.1.2.8 Cyclohexanone</td>
<td>2660</td>
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<td>12.1.2.9 Acetophenone</td>
<td>2664</td>
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<td>12.1.2.10 Benzophenone</td>
<td>2670</td>
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<td>2673</td>
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<td>2679</td>
</tr>
</tbody>
</table>
12.1 LIST OF CHEMICALS AND DATA COMPILATIONS

12.1.1 ALDEHYDES

12.1.1.1 Methanal (Formaldehyde)

Common Name: Formaldehyde
Synonym: formalin, methanal, oxomethane
Chemical Name: formaldehyde
CAS Registry No: 50-00-0
Molecular Formula: CH₂O, HCHO
Molecular Weight: 30.026
Melting Point (°C):
  -92.0 (Weast 1982–83; Dean 1985; Lide 2003)
Boiling Point (°C):
  -19.1 (Lide 2003)
Density (g/cm³):
  0.815 (–20°C, Weast 1982–83)
  0.815 (–20°C, Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
  36.8 (–20°C, Stephenson & Malanowski 1987)
  29.6 (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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  1220000 (Dean 1985)
  very soluble, up to 55% (Budavari 1989, Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  101325* (–19.5°C, summary of literature data, temp range –88 to –19.5°C, Stull 1947)
  log (P/mmHg) = [–0.2185 × 5917.9/(T/K)] + 7.985746; temp range –88 to –19.5°C (Antoine eq., Weast 1972–73)
  1333 (–88°C, Verschueren 1983)
  log (P/kPa) = 6.32524 – 972.5/(244.329 + t°C), temp range (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  log (P/mmHg) = 7.1958 – 970.65/(244.1 + t°C); temp range –109 to –22°C (Antoine eq., Dean 1985, 1992)
  log (P₁/kPa) = 6.5475 – 1062.4/(-19.92 + T/K), temp range 184–251 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P₁/kPa) = 6.4306 – 1013.206/(-24.883 + T/K); temp range 163–251 K (Antoine eq.-II, Stephenson & Malanowski 1987)
  517690 (1 atm, Howard 1989)
  log (P/mmHg) = 41.9603 – 2.1355 × 10³/(T/K) – 13.765 log (T/K) + 9.568 × 10⁻³(T/K) – 5.1101 × 10⁻¹²(T/K)²;
  temp range 181–408 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.0331 (20°C, porous membrane gas-liquid equilibration system, Dong & Dasgupta 1986)
  0.0169 (review, Gaffney et al. 1987)
  0.0341* (gas stripping-headspace GC, measured range 15–45°C, Betterton & Hoffmann 1988)
0.0298* (gas-stripping-HPLC-UV, freshwater, measured range 10–45°C, Zhou & Mopper 1990)
In [K\textsubscript{H}′/(M/atm)] = −6.0 + 2844/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
In [K\textsubscript{H}′/(M/atm)] = −6.7 + 3069/(T/K), temp range 25–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1‰), Zhou & Mopper 1990)
0.021 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K\textsubscript{AW} = 4.621 − 2840/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K\textsubscript{ow}:
- 0.35 (shake flask, Johnson & Piret 1948)
- 1.54 (Kenaga & Goring 1980)
- 0.00 (Verschueren 1983)
- 0.35 (recommended, Sangster 1989)
- 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K\textsubscript{oa}:

Bioconcentration Factor, log BCF:
- no bioconcentration. in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, log K\textsubscript{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t\textsubscript{1/2}:
Volatilization:
Photolysis: sunlight photolysis t\textsubscript{1/2} = 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);
rate constant k = 8.0 × 10\textsuperscript{−5} s\textsuperscript{−1} in the atmosphere (Carlier et al. 1986);
calculated lifetime of 4 h (Atkinson 2000).
Oxidation: rate constant k, for gas-phase second order rate constants, k\textsubscript{OH} for reaction with OH radical, k\textsubscript{NO3} with NO\textsubscript{3} radical and k\textsubscript{O3} with O\textsubscript{3} or as indicated, *data at other temperatures and/or Arrhenius equation see reference:
k\textsubscript{OH} = 1.4 × 10\textsuperscript{−11} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at 298 K (discharge flow system-MS, Morris & Niki 1971)
aqueous photooxidation t\textsubscript{1/2} = 4813–190000 h, based on measured rate constant for the reaction with OH radical in water (Dorfan & Adams 1973; quoted, Howard et al. 1991)
k\textsubscript{OH} = 1.5 × 10\textsuperscript{−11} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} (long-path Fourier transform IR, Niki et al. 1978)
k\textsubscript{NO3} = 3.2 × 10\textsuperscript{−16} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at 298 ± 1 K (review, Atkinson & Lloyd 1984)
k = (0.1 ± 0.03) M\textsuperscript{−1} s\textsuperscript{−1} for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)
k\textsubscript{HO2} = 4.5 × 10\textsuperscript{−14} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} for the vapor-phase reaction with HO\textsubscript{2} radical at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)
k\textsubscript{OH} = 1.1 × 10\textsuperscript{−11} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)
k\textsubscript{OH(calc)} = 7.4 × 10\textsuperscript{−12} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1}, k\textsubscript{OH(obs.)} = 9.0 × 10\textsuperscript{−12} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at room temp. (SAR structure-activity relationship, Atkinson 1985)
atmospheric photooxidation half-life of 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)
k\textsubscript{OH*} = 9.77 × 10\textsuperscript{−12} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at 298 K (recommended, Atkinson 1989)
k\textsubscript{NO3} = 5.8 × 10\textsuperscript{−16} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} at 298 K (recommended, Atkinson 1991)
k\textsubscript{OH(calc)} = 17.5 × 10\textsuperscript{−15} cm\textsuperscript{3} molecule\textsuperscript{−1} s\textsuperscript{−1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable group (Howard et al. 1991).
Biodegradation: degradation complete in 20 h under aerobic conditions and 48 h under anaerobic conditions in a die-away test using water from a stagnant lake (Howard 1989)
aqueous aerobic half-life of 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data; aqueous anaerobic half-life of 96–672 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: half-life is a few hours in the sunlit troposphere; $t_{1/2} = 19$ and $50$ h by dry deposition and wet removal, respectively; $t_{1/2} = 12$ d when reacts with NO$_3$ radical by H-atom abstraction. (Howard 1989)
   photooxidation $t_{1/2} = 7.13$–$71.3$ h, based on measured rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);
   $t_{1/2} = 1.26$–$6.0$ h, based on photolysis half-life in air (Howard et al. 1991);
   atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);
   calculated lifetimes of 1.2 d, 80 d and > 4.5 yr for reactions with OH radical, NO$_3$ radical and O$_3$, respectively (Atkinson 2000).

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

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

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

   Biota:

<table>
<thead>
<tr>
<th>Table 12.1.1.1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of methanal (formaldehyde) at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

$$
\begin{align*}
\text{Spencer & Wild 1935} & \\
 & \text{differential manometer} & \text{Stull 1947} & \text{summary of literature data} \\
\text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} \\
-109.39 & 127 & -88.0 & 1333 & -92 & mp/°C \\
-104.39 & 237 & -79.6 & 2666 & - & -22.9 & 88566 \\
-98.29 & 480 & -70.6 & 5333 & - & -28.39 & 66208 \\
-95.19 & 647 & -65.0 & 7999 & - & -34.29 & 49182 \\
-89.09 & 1157 & -57.3 & 13332 & - & -39.09 & 38743 \\
-85.59 & 1633 & -46.0 & 26664 & - & -34.29 & 101325 \\
-78.89 & 2802 & -33.0 & 53329 & - & -71.29 & 4720 \\
-78.29 & 2946 & -19.5 & 101325 & - & -68.55 & 6190 \\
-71.29 & 4720 & - & -22.29 & 88566 \\
-68.59 & 7859 & - & -28.39 & 66208 \\
-64.59 & 8219 & - & -34.29 & 49182 \\
-63.69 & 8693 & - & -39.09 & 38743 \\
-55.79 & 14799 & - & -49.29 & 21745 \\
-53.99 & 16625 & - & -40.59 & 35544 \\
-49.29 & 21745 & - & -39.09 & 38743 \\
-42.29 & 49182 & - & -34.29 & 101325 \\
-22.29 & 88566 & - & -22.29 & 88566 \\
\end{align*}
$$

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Aldehydes and Ketones

FIGURE 12.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanal.

TABLE 12.1.1.1.2
Reported Henry’s law constants of methanal (formaldehyde) at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th></th>
<th>$\ln K_{AW} = A - B/(T/K)$</th>
<th>$\log K_{AW} = A - B/(T/K)$</th>
<th>$\ln (1/K_{AW}) = A - B/(T/K)$</th>
<th>$\log (1/K_{AW}) = A - B/(T/K)$</th>
<th>$\ln [H/(Pa \cdot m^3/mol)] = A - B/(T/K)$</th>
<th>$\ln [H/(atm \cdot m^3/mol)] = A - B/(T/K)$</th>
<th>$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Betterton &amp; Hoffmann 1988</td>
<td>fresh water</td>
<td>$0.01386$</td>
<td>$0.01023$</td>
<td>$0.0074$</td>
<td>$0.0128$</td>
<td>$0.01023$</td>
<td>$0.0074$</td>
</tr>
<tr>
<td>Zhou &amp; Mopper 1990</td>
<td>sea water</td>
<td>$0.01031^*$</td>
<td>$0.0298$</td>
<td>$0.0284$</td>
<td>$0.1506$</td>
<td>$0.0533$</td>
<td>$-0.0284$</td>
</tr>
<tr>
<td>t/°C</td>
<td>$H/(Pa \cdot m^3/mol)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>$0.01386$</td>
<td>15</td>
<td>$0.01023$</td>
<td>10</td>
<td>$0.0074$</td>
<td>$0.0128$</td>
<td>$0.01023$</td>
</tr>
<tr>
<td>25</td>
<td>$0.0341$</td>
<td>25</td>
<td>$0.0298$</td>
<td>25</td>
<td>$0.0284$</td>
<td>$0.0298$</td>
<td>$0.0284$</td>
</tr>
<tr>
<td>35</td>
<td>$0.0675$</td>
<td>30</td>
<td>$0.0507$</td>
<td>30</td>
<td>$0.0405$</td>
<td>$0.0507$</td>
<td>$0.0405$</td>
</tr>
<tr>
<td>45</td>
<td>$0.1506$</td>
<td>40</td>
<td>$0.0921$</td>
<td>40</td>
<td>$-0.0284$</td>
<td>$0.0921$</td>
<td>$-0.0284$</td>
</tr>
<tr>
<td>$\Delta H/(kJ \cdot mol^{-1}) = -59.8$</td>
<td>$0.1506$</td>
<td>45</td>
<td>$0.125$</td>
<td>45</td>
<td>$0.115$</td>
<td>$0.125$</td>
<td>$0.115$</td>
</tr>
<tr>
<td>* in 0.5 M HSO₄ solution</td>
<td>$\log K_A'$/(M/atm)</td>
<td>eq. 1a</td>
<td>$K_A'$/(M/atm)</td>
<td>eq. 1a</td>
<td>$K_A'$/(M/atm)</td>
<td>eq. 1a</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>$-6.00$</td>
<td>A</td>
<td>$-6.00$</td>
<td>A</td>
<td>$-6.00$</td>
<td>A</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>$-2844$</td>
<td>B</td>
<td>$-2844$</td>
<td>B</td>
<td>$-3069$</td>
<td>B</td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 12.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanal.
12.1.1.2 Ethanal (Acetaldehyde)

Common Name: Acetaldehyde
Synonym: acetic aldehyde, aldehyde, ethanal, ethylaldehyde
Chemical Name: acetaldehyde, ethanal
CAS Registry No: 75-07-0
Molecular Formula: C₂H₄O, CH₃CHO
Molecular Weight: 44.052
Melting Point (°C): –123.37 (Lide 2003)
Boiling Point (°C): 20.1 (Lide 2003)
Density (g/cm³ at 20°C): 0.7834 (18°C, Lide 2003)
Molar Volume (cm³/mol):
56.23 (18°C, calculated-density)
51.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
–10.2 (pKₐ, Riddick et al. 1986)
Enthalpy of Fusion ∆Hₘₙₜ (kJ/mol):
3.243 (Riddick et al. 1986)
Entropy of Fusion ∆Sₘₙₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₘₙₜ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Palit 1947; Riddick et al. 1986)
miscible (Verschueren 1983; Dean 1985)
miscible (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):
101300* (20.2°C, summary of literature data, temp range –81.5 to 5.9°C, Stull 1947)
102125* (20.7°C, measured range –0.2 to 34.4°C, Coles & Popper 1950)
120060 (Hoy 1970)
log (P/mmHg) = [−0.2185 × 7267.8/(T/K)] + 8.327803; temp range –81.5 to 20.2°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = [−0.2185 × 6622.1/(T/K)] + 7.82060; temp range –24.3 to 27.5°C (Antoine eq., Weast 1972–73)
98640 (20°C, Verschueren 1983)
102125, 120220 (20.7°C, quoted exptl., interpolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 7.14122 – 1606.85/(292.482 + t°C), temp range: –0.2 to 34.3°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
120230 (calculated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 8.00552 – 1600.017/(291.809 + t°C), temp range: liquid (Antoine eq., Dean 1985, 1992)
121300 (selected, Riddick et al. 1986)
log (P/kPa) = 6.1814 – 1070.6/(236.0 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
120700 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P₁/kPa) = 6.1410 – 1034.5/(–43.15 + T/K); temp range 272–294 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P₁/kPa) = 6.03292 – 1012.828/(–41.823 + T/K); temp range 293–377 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/mmHg) = 87.3702 – 3.6822 × 10³/(T/K) – 31.548 log (T/K) + 2.0114 × 10⁻²(T/K) + 5.5341 × 10⁻¹(T/K)²; temp range 150–461 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.692 (shake flask-concentration ratio-GC, Buttery et al. 1969)
8.924 (calculated K_{AW}, Buttery et al. 1969)
6.672 (exptl., Hine & Mookerjee 1975)
5.946, 5.423 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1.336, 8.0 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
6.75 (review, Gaffney et al. 1987)
2.578* (gas stripping-headspace GC, measured range 15–35°C, Betterton & Hoffmann 1988)
6.80* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
ln [K_{f}′/(M/atm)] = –6.03 + 276/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
ln [K_{f}′/(M/atm)] = –5.21 + 1984/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1‰), Zhou & Mopper 1990)
10.18 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
5.47* (20°C, headspace-GC, measured range 10–40°C, Benkelberg et al. 1995)
8.72* (headspace-GC, artificial seawater, measured range 16–40°C, Benkelberg et al. 1995)
ln (k_{f}′/atm) = (20.4 ± 0.1) – (5671 ± 22)/(T/K); temp range 10–40°C (headspace-GC measurements, Benkelberg et al. 1995)
5.14 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
6.33 (solid-phase microextraction SPME-GC, Bartelt 1997)
6.69 (equilibrium headspace-GC, Marin et al. 1999)
5.39 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 5.324 – 2340/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
0.52 (generator column-HPLC, Wasik et al. 1981)
0.36 (generator column-GC, Tewari et al. 1982)
0.43 (calculated, Verschueren 1983)
0.45 (recommended, Sangster 1989, 1993)

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

Bioconcentration Factor, log BCF

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization:
Photolysis: rate constant k = 2.3.0 × 10⁻⁵ s⁻¹ in the atmosphere (Carlier et al. 1986); calculated lifetime of 6 d (Atkinson 2000)
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures and or Arrhenius equation see reference:
k_{OH} = 1.53 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (discharge flow system-MS, Morris & Niki 1971)
k_{OH} = 1.6.2 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ (long-path Fourier transform IR, Niki et al. 1978)
k = 0.1 M⁻¹ s⁻¹ for oxidation by RO₂ radical at 30°C in aquatic systems with half-life of 8 × 10⁴ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
k < 2 × 10³ M⁻¹ s⁻¹ for oxidation by singlet oxygen at 25°C in aquatic systems with half-life > 00 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
k_{OH} = (12.8 ± 4.3) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (Kerr & Sheppard 1981; quoted, Atkinson 1985)
k = (1.5 ± 0.2) M⁻¹ s⁻¹ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)
k_{OH} = (12.2 ± 2.7) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Sémmes et al. 1985; quoted, Atkinson 1985)
k_{O₃} = (3.4 ± 0.5) × 10⁻³⁰ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (Stedman & Niki 1973; quoted, Atkinson & Carter 1984)
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$k_{OH} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k_{O3} \leq 6 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K}$ (Atkinson et al. 1981, 1982; quoted, Atkinson & Carter 1984; Atkinson 1985)

$k_{HO2} = 1.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with HO$_2$ radical at 293 K in the atmosphere (Barnes et al. 1982; quoted, Carlier et al. 1986)

$k_{OH} = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{NO3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in air (Atkinson et al. 1984)

$k_{NO3} = 1.40 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 1 \text{ K}$ (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{OH} = 1.60 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{OH} = (14.7 \pm 2.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Michael et al. 1985; quoted, Atkinson 1985)

$k_{OH}^{\text{(calc)}} = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}^{\text{(obs.)}} = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 1.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d$^{-1}$, $k_{O3} \leq 6.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.0004 d$^{-1}$, $k_{NO3} = 2.5 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.05 d$^{-1}$ (review, Atkinson 1985)

$k_{OH}^{\#} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 16.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{NO3} = 2.78 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH} = 10.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

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

Half-Lives in the Environment:

Air: $t_h < 0.24 \text{ h}$ 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); atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994); calculated lifetimes of 8.8 h, 17 d and $> 4.5 \text{ yr}$ for reactions with OH radical, NO$_3$ radical and O$_3$, respectively (Atkinson 2000).

Surface water:
Ground water:
Sediment:
Soil:
Biota:
TABLE 12.1.1.2.1
Reported vapor pressures of ethanal (acetaldehyde) at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947
Coles & Popper 1950

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>-81.5</td>
<td>133.3</td>
<td>-0.20</td>
<td>44263</td>
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<tr>
<td>-65.1</td>
<td>666.6</td>
<td>2.70</td>
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<td>-56.8</td>
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<td>11.6</td>
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<td>90926</td>
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<td>-10.0</td>
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<td>20.7</td>
<td>102125</td>
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<td>4.90</td>
<td>53329</td>
<td>30.8</td>
<td>149321</td>
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<tr>
<td>20.2</td>
<td>101325</td>
<td>34.4</td>
<td>167852</td>
</tr>
<tr>
<td>mp/°C</td>
<td>-123.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

mp/°C = -123.5
b.p/°C = 20.4

Equation
A
B

Ethanal (acetaldehyde): vapor pressure vs. 1/T

FIGURE 12.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethanal.
TABLE 12.1.1.2.2
Reported Henry's law constants of ethanal (acetaldehyde) at various temperatures and temperature
dependence equations

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

1.

<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>gas stripping-GC</td>
<td>gas stripping-GC, spec.</td>
<td>gas stripping-HPLC/UV</td>
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<td>( t/°C )</td>
<td>( H/(\text{Pa m}^3/\text{mol}) )</td>
<td>( t/°C )</td>
</tr>
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<td>fresh water</td>
<td>sea water</td>
<td>fresh water</td>
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<tr>
<td>0</td>
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<td>25</td>
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<tr>
<td></td>
<td></td>
<td>35</td>
</tr>
<tr>
<td>enthalpy of transfer:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Delta H/(\text{kJ mol}^{-1}) = -46.024 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>15.446</td>
<td>35</td>
</tr>
<tr>
<td>40</td>
<td>-</td>
<td>40</td>
</tr>
<tr>
<td>45</td>
<td>15.59</td>
<td>45</td>
</tr>
<tr>
<td>eq. 1</td>
<td>( K_H/\text{M/atm} )</td>
<td>eq. 1</td>
</tr>
<tr>
<td>A</td>
<td>-6.03</td>
<td>A</td>
</tr>
<tr>
<td>B</td>
<td>-2164</td>
<td>B</td>
</tr>
</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>Benkelberg et al. 1995</th>
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<tbody>
<tr>
<td>equilibrium vapor phase concentration-headspace GC</td>
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<tr>
<td>( t/°C )</td>
</tr>
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<td>deionized water</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>15</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>for deionized and rain water:</td>
</tr>
<tr>
<td>eq. 3</td>
</tr>
<tr>
<td>A</td>
</tr>
<tr>
<td>B</td>
</tr>
<tr>
<td>( \Delta H/(\text{kJ mol}^{-1}) = -47.15 )</td>
</tr>
</tbody>
</table>
FIGURE 12.1.1.2.2 Logarithm of Henry’s law constant versus reciprocal temperature for ethanal.
12.1.1.3 Propanal (Propionaldehyde)

Common Name: Propionaldehyde
Synonym: propanal
Chemical Name: propionaldehyde, propanal
CAS Registry No: 123-38-6
Molecular Formula: C₃H₆O, CH₃CH₂CHO
Molecular Weight: 58.079
Melting Point (°C):
-80 (Lide 2003)
Boiling Point (°C):
48 (Lide 2003)
Density (g/cm³ at 20°C):
0.8058 (Weast 1982–83)
0.7970 (Riddick et al. 1986)
Molar Volume (cm³/mol):
72.9 (calculated-density, Stephenson & Malanowski 1987)
74.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion ∆Hₘ (kJ/mol):  
Entropy of Fusion ∆Sₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₘ = 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):
160000 (20°C, Seidell 1941)
200000 (20°C, Verschueren 1983)
306000 (Dean 1985; Riddick et al. 1986)
405000 (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):
67661* (39.07°C, ebulliometry, measured range 39.07–50.29°C, Dreisbach & Shrader 1949)
log (P/mmHg) = 7.08683 – 1178.9/(230 + t°C); temp range not specified (Antoine eq., Dreisbach & Martin 1949)
42340 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.2902 – 1210.87/(234.65 + t°C), temp range 13.1–48.06°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1974, Boublik et al. 1984)
42490, 42360 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)
log (Pᵢ/kPa) = 6.2047 – 1166.99/(–43.15 + T/K); temp range 290–322 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (Pᵢ/kPa) = 6.2336 – 1180/(–42.0 + T/K); temp range 250–330 K (Antoine eq.-II, Stephenson & Malanowski 1987)
23190 (calculated-solvatochromic parameters, Banerjee et al. 1990)
log (P/mmHg) = 26.1637 – 2.3059 × 10³/(T/K) – 6.5289 log (T/K) – 2.3065 × 10⁻⁹(T/K) + 2.5454 × 10⁻⁶(T/K)²; temp range 193–496 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
7.436 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
7.486 (exptl., Hine & Mookerjee 1975)
8.40, 8.21 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
8.305 " (gas stripping-HPLC/UV, measured range 10–45°C, Zhou & Mopper 1990)
ln [K_H′(M/atm)] = –7.15 + 2467/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
ln [K_H′(M/atm)] = –6.60 + 2273/(T/K), temp range 25–35°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1), Zhou & Mopper 1990)
7.486, 13.62 (quoted, correlated-molecular structure, Russell et al. 1992)
5.48 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.324 – 2237/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
0.83 (calculated, Verschueren 1983)
0.59 (shake flask, Log P Database, Hansch & Leo 1987)
0.59 (recommended, Sangster 1989)
0.59 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
3.02 (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: rate constant $k = 3.2 \times 10^{-5}$ s$^{-1}$ in the atmosphere (Carlier et al. 1986).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH} = 3.06 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)
photooxidation $t_{1/2}$ < 0.24 h for the gas-phase reaction with OH radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)
$k_{OH} = 2.1 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)
$k_{OH} = (18.5 \pm 2.1) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Audley et al. 1981; quoted, Atkinson 1985),
$k_{OH} = (19.5 \pm 1.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Kerr & Sheppard 1981; quoted, Atkinson 1985)
$k = (2.5 \pm 0.4)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)
$k_{OH} = 1.8 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)
$k_{OH} = (17.1 \pm 2.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)
$k_{OH(calc)} = 2.2 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH(obs.)} = 1.96 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)
photooxidation $t_{1/2}$ = 3.3–33 h in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991)
$k_{OH} = 1.96 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
$k_{OH(calc)} = 16.55 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: biodegradation rate constants $k = 0.046–0.063$ h$^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Uran & Kato 1986b); aqueous aerobic $t_{1/2} = 24–168$ h, based on aerobic biological screening test data (Gerhold & Malaney 1966; Dore et al. 1975; Uran & Kato 1986; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96–672$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

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

Half-Lives in the Environment:
Air: $t_{1/2} < 0.24$ h 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);
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...photooxidation $t_{\text{1/2}} = 3.3–33$ h in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

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

Ground water: $t_{\text{1/2}} = 48–336$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

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

Biota:

### TABLE 12.1.1.3.1

Reported aqueous solubilities and vapor pressures of propanal (propionaldehyde) at various temperatures

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<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
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<td><strong>Stephenson 1993</strong></td>
<td><strong>Dreisbach &amp; Shrader 1949</strong></td>
</tr>
<tr>
<td></td>
<td>shake flask-GC/TC</td>
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<tr>
<td></td>
<td>$t/{}^\circ C$</td>
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<tr>
<td>12.3</td>
<td>477000</td>
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**FIGURE 12.1.1.3.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propanal.
TABLE 12.1.1.3.2
Reported Henry’s law constants of propanal (propionaldehyde) at various temperatures and temperature dependence equations

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

Zhou & Mopper 1990

gas stripping-HPLC/UV \hspace{2cm} \hspace{2cm} \hspace{2cm} \text{gas stripping-HPLC/UV}

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FIGURE 12.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for propanal.
FIGURE 12.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for propanal.
12.1.1.4 Butanal (n-Butyraldehyde)

Common Name: n-Butyraldehyde
Synonym: 1-butanal, butyraldehyde, butyric aldehyde
Chemical Name: butyraldehyde, butanal
CAS Registry No: 123-72-8
Molecular Formula: C₄H₈O, CH₃CH₂CH₂CHO
Molecular Weight: 72.106
Melting Point (°C): ~96.86 (Lide 2003)
Boiling Point (°C): 74.8 (Lide 2003)
Density (g/cm³ at 20°C):
0.8170 (Weast 1982–83; Verschueren 1983)
0.8016 (Dean 1985; Riddick et al. 1986)
Molar Volume (cm³/mol):
90.0 (20°C, calculated-density)
96.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion $\Delta H_{\text{fus}}$ (kJ/mol):
11.088 (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/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
36000 (20°C, quoted, Palit 1947)
37840 (Deno & Berkheimer 1960)
37000, 71000 (lit. values, Verschueren 1983)
71000 (Dean 1985; Riddick et al. 1986)
83700 (selected, Yaws et al. 1990)
74400*, 54800 (20°C, 30°C, shake flask-GC/TC, measured range 0–70°C, Stephenson 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):
19372* (30.71°C, measured range 30.71–74.03°C, Seprakova et al. 1959; quoted, Boublík et al. 1984)
9464 (20°C, Verschueren 1983)
14798 (extrapolated-Antoine eq., Boublík et al. 1984)
$\log (P/\text{kPa}) = 5.52728 - 921.802/(186.564 + t/°C)$; temp range 30.71–74.03°C (Antoine eq. from reported exptl. data of Seprakova et al. 1959, Boublík et al. 1984)
14785 (extrapolated-Antoine eq., Dean 1985)
$\log (P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/°C)$; temp range ~87 to 7°C (Antoine eq., Dean 1985, 1992)
15700 (selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.1461 - 1233.0/(223.0 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
14780 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P/\text{kPa}) = 5.68618 - 994.1/(-78.05 + T/K)$; temp range 293–349 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P/\text{kPa}) = 5.40874 - 1182.472/(T/K)$; temp range 348–423 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 66.8411 - 3.6784 \times 10^3/(T/K) –22.609 \log (T/K) + 1.1697 \times 10^{-2}(T/K) + 2.9647 \times 10^{-13}(T/K)^2$; temp range 177–525 K (vapor pressure eq., Yaws 1994)
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):

11.65 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
11.65 (gas stripping-HPLC, Zhou & Mopper 1990)

\[ \ln \left[ \frac{K_H}{(M/\text{atm})} \right] = -8.07 + \frac{2701}{(T/K)}; \text{ temp range 10–45°C} \]

\[ \ln \left[ \frac{K_H}{(M/\text{atm})} \right] = -8.20 + \frac{2698}{(T/K)}; \text{ temp range 10–45°C} \]

7.26 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

\[ \log K_{\text{AW}} = 6.244 - \frac{2571}{(T/K)} \]

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

1.20 (Hansch & Leo 1979)
0.88 (shake flask, Log P Database, Hansch & Leo 1987)
0.88 (recommended, Sangster 1989)
0.88 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

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

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

Volatileization:

Photolysis: rate constant $k = 2.7 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986)

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

photooxidation $t_{1/2} = 114 \text{ d to 19 yr}$ in water, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{\text{OH}} = (26.2 \pm 3.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Audley et al. 1981; quoted, Atkinson 1985)

$k_{\text{OH}} = (25.3 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k_{\text{OH}} = 25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k = (2.5 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}} = (30.8 \pm 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence technique. Semmes et al. 1985; quoted, Atkinson 1985)

$k_{\text{OH(calc)}} = 2.55 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH(obs.)}} = 2.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 2.8$–28 h in air, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{\text{OH}} = 2.35 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: rate constants $k = 0.044$–0.069 h$^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Uran & Kato 1986b);
aqueous aerobic $t_{1/2} = 24–168$ h, based on aerobic biological screening test data (Lamb & Jenkins 1952; Heukelekian & Rand 1955; Dore et al. 1975; Urano & Kato 1986b; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96–672$ 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 $t_{1/2} = 2.8–28$ h, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
calculated lifetimes of 5.9 d for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 114$ d to 19 yr, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991);

$\text{bp/°C} = 75$

$\log P = A - B/(C + t/°C)$
eq 2

$A \quad 5.52728$
$B \quad 921.802$
$C \quad 186.564$
$\text{bp/°C} \quad 75.195$
$\text{eq in Boublík et al. 1984}$
Aldehydes and Ketones

FIGURE 12.1.1.4.1 Logarithm of mole fraction solubility (ln \(x\)) versus reciprocal temperature for butanal.

TABLE 12.1.1.4.2
Reported Henry’s law constants of butanal (\(n\)-butyraldehyde) at various temperatures and temperature dependence equations

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

Zhou & Mopper 1990

gas stripping-HPLC/UV
gas stripping-HPLC/UV

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<th>(H/(Pa \cdot m^3/mol))</th>
<th>(t^\circ C)</th>
<th>(H/(Pa \cdot m^3/mol))</th>
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FIGURE 12.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for butanal.

FIGURE 12.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for butanal.
12.1.1.5 2-Propenal (Acrolein)

Common Name: Acrolein
Synonym: 2-propanal, acraldehyde, acrylic aldehyde, allyaldehyde, acrylaldehyde, aqualin
Chemical Name: 2-propanal
CAS Registry No: 107-02-8
Molecular Formula: C₃H₄O, CH₂=CHCHO
Molecular Weight: 56.063
Melting Point (°C):
   -87.7  (Lide 2003)
Boiling Point (°C):
   52.6   (Lide 2003)
Density (g/cm³ at 20°C):
   0.8389 (Riddick et al. 1986)
Dissociation Constant:
Molar Volume (cm³/mol):
   66.8  (20°C, calculated-density)
   66.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘ₀ (kJ/mol):
Entropy of Fusion, ΔSₘ₀ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘ₀ = 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):
   208000  (20°C, Günther et al. 1968; Callahan et al. 1979; Verschueren 1977, 1983)
   102020  (shake flask-radioactive analysis, Veith et al. 1980)
   208000  (selected, Riddick et al. 1986)
   229000*, 230000 (20°C, 30°C, shake flask-GC/TC, measured range 0–53°C, Stephenson 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):
   26664*  (17.5°C, summary of literature data, temp range –64.5 to 52.5°C, Stull 1947)
   log (P/mmHg) = [–0.2185 × 7628.8/(T/K)] + 8.033866; temp range: –64.5 to 52.5°C, (Antoine eq., Weast 1972–73)
   35300  (Riddick et al. 1986, Howard 1989)
   36610, 35360 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
   log (P/Pₐ) = 6.19181 – 1204.9/(–37.8 + T/K); temp range 208–326 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P/Pₐ) = 6.2878 – 1231.003/(–38.405 + T/K); temp range 250–306 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P/mmHg) = 57.9815 – 3.093×10³/(T/K) – 19.638·log (T/K) + 1.1486·10⁻²·(T/K)²; temp range 185–506 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
   2.84, 13.77  (0, 25°C, headspace-GC, Snider & Dawson 1985)
   12.36  (review, Gaffney et al. 1987)
   0.446  (Howard 1989)
   5.48  (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
   log Kₐw = 4.823 – 2110/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log Kₐw:
   –0.09  (quoted, Callahan et al. 1979)
   0.90  (measured value, Veith et al. 1980)
Octanol/Air Partition Coefficient, log $K_{OA}$:

-0.10 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Sangster 1993)
-0.01 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.54 (bluegill sunfish, Barrows et al. 1980)
2.54 (bluegill sunfish, Veith et al. 1980)
-0.22 (estimated-$K_{OW}$, Howard 1989)

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

1.38 (estimated-$K_{OW}$, Howard et al. 1989)
-0.219 (calculated-$K_{OW}$, Kollig 1993)

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

Volatilization: $t_{1/2} = 10$ d from a model river (Howard 1989);
Photolysis: $t_{1/2} = 3.5$ d, based on measured quantum yields (Howard 1989).
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{O3} = 6.4 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson & Carter 1984)
- $k_{OH} = (1.90 - 2.53) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in air (Atkinson 1985)
- $k_{OH} = 20.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 23.5°C using propylene as reference compound, with a atmospheric lifetime of 0.56 d (Edney et al. 1986)
- $k_{NO3} = 5.9 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated atmospheric lifetime of 16 d, $k_{OH} = 2.0 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a lifetime of 1.2 d; and $k_{O3} = 2.8 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a lifetime of 59 d at room temp. (Atkinson et al. 1987)
- $k_{OH}(calc) = 2.29 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 1.96 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
- $k_{OH} = 1.99 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
- atmospheric $t_{1/2} = 3.4$–33.7 h, based on rate constant for reaction with OH radical (Howard et al. 1991)
- $k_{OH} = 22.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO3} = 1.15 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ ((Sabljic & Güsten 1990; Müller & Klein 1991)
- $k_{OH}(calc) = 17.70 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Callahan et al. 1979).

Biodegradation: $t_{1/2} = 29$ h (natural unsterilized water) and $t_{1/2} = 43$ h in sterilized (thymol-treated) water (Bowmer & Higgins 1976, quoted, Howard 1989);
aqueous aerobic $t_{1/2} = 168$–672 h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2} = 672$–2880 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $t_{1/2} < 4$ d (Callahan et al. 1979)

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

Half-Lives in the Environmental Compartments:

Air: atmospheric lifetime of 0.56 d due to reaction with OH radical (Edney et al. 1986);
calculated atmospheric lifetimes: 16 d for reaction with NO$_3$ radical, 1.2 d with OH radical and 59 d with O$_3$ (Atkinson et al. 1987);
- $t_{1/2} = 10$–13 h for reaction with photochemically generated hydroxyl radical, $t_{1/2} = 18$ d for reaction with ozone and $t_{1/2} = 3.5$ d for photodissociation in the atmosphere (Howard 1989);
- $t_{1/2} = 3.4$–33.7 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: removal $t_{1/2} = 2.0$ to 2.5 d from water (Howard 1989);
First order $k = 0.163$ h$^{-1}$ in 8 agricultural canals and varies between 0.104 and 0.211 h$^{-1}$ at pH 7.1 to 7.5 and water temperature of 16–24°C, the mean value corresponds to $t_{1/2} = 4.25$ h at 21°C (Bowmer & Sainty 1977)

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aqueous aerobic $t_{1/2} = 168–672$ h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2} = 672–2880$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991) 

$k = 0.015$ h$^{-1}$ at 21°C and pH 7.0, corresponding to $t_{1/2} = 46$ h in dilute buffered solutions of acrolein in distilled water. (Nordone et al. 1996) 

Dissipation $k = 0.068$ h$^{-1}$ with $t_{1/2} = 10.2$ h and $k = 0.028$ h$^{-1}$ with $t_{1/2} = 7.3$ h in weedy (Pump Canal, 12–20°C) and non-weedy agricultural canals (Lateral 1, 12–18°C), respectively, dissipation is the result of numerous processes including degradation, volatilization, adsorption and dilution (Nordone et al. 1996) 

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

Sediment: 
Soil: $t_{1/2} = 168–672$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991). 

Biota:

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<td>$t/°C$</td>
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**FIGURE 12.1.1.5.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-propenal.
FIGURE 12.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-propenal.
12.1.1.6 Furfural (2-Furaldehyde)

Common Name: Furfural
Synonym: 2-furaldehyde, 2-furancarboxaldehyde; furfurole, 2-furancarbonal, fural, furfuraldehyde, furole
Chemical Name: furfural
CAS Registry No: 98-01-1
Molecular Formula: C₅H₄O₂
Molecular Weight: 96.085
Melting Point (°C):
   −38.1 (Lide 2003)
Boiling Point (°C):
   161.7 (Lide 2003)
Density (g/cm³ at 20°C):
   1.16 (Verschueren 1983)
Dissociation Constant:
Molar Volume (cm³/mol):
   82.9 (calculated-density, Stephenson & Malanowski 1987)
   92.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, Δ_Hfus (kJ/mol):
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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
   82000 (40°C, synthetic method, Jones 1929)
   91593 (shake flask-volumetric method, Booth & Everson 1948)
   92900 (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
   77830 (generator column-HPLC/UV, Tewari et al. 1982)
   79400*, 84000 (20°C, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 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):
   1066.6* (39.9°C, ebulliometry, measured range 40–170.6°C, Evans & Aylesworth 1926)
   220.4* (interpolated-regression of tabulated data, temp range 18.5–161.8°C, Stull 1947)
   1767* (55.6°C, Ramsay-Young method, measured range 55.6–170°C, Matthews et al. 1950)
   log (P/mmHg) = A – B/(T/K) – C log (T/K); temp range 55.6–170°C (Kirchhoff eq., Matthews et al. 1950)
   log (P/mmHg) = [−0.2185 × 11614.6/(T/K)] + 8.729884; temp range 18.5–161.8°C (Antoine eq., Weast 1972–73)
   133.3, 400 (20°C, 30°C, Verschueren 1983)
   log (P/kPa) = 5.62941 – 1124.58/(148.82 + t°C), temp range 92.3–170.6°C (Antoine eq. derived from Evans & Aylesworth 1926 data, Boublik et al. 1984)
   log (P/kPa) = 5.76606 – 1236.74/(167.368 + t°C), temp range 55.87–160.8°C (Anotoine eq. derived from Matthews et al. 1950 data, Boublík et al. 1984)
   208.0 (extrapolated-Antoine eq., Dean 1985)
   log (P/mmHg) = 6.91048 – 946.35/(246.68 + t°C), temp range 87 to 7°C (Antoine eq., Dean 1985, 1992)
   333.3 (Riddick et al. 1986)
   313.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
   log (P/kPa) = 6.41784 – 1663.16/(−57.88 + T/K), temp range 357–435 K (Antoine eq., Stephenson & Malanowski 1987)
   log (P/mmHg) = 32.0337 – 3.3161 × 10^3/(T/K) + 10.171 log (T/K) – 2.1115 × 10^2,(T/K) + 9.2045 × 10^6(T/K)^2; temp range 237–657 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa-m³/mol):
   0.375 (calculated-P/C, Howard 1993)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 0.34 (20°C, shake flask, Korenman 1972)
- 0.52 (generator column-HPLC/UV, Tewari et al. 1982)
- 0.41, 0.52 (shake flask, Log P Database, Hansch & Leo 1987)
- 0.46 (recommended, Sangster 1993)
- 0.41 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log $BCF$:
- 0.079 (estimated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1993)
- −2.097 (estimated-$S$, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log $K_{OC}$:
- 1.602 (soil, estimated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1993)
- 0.00 (soil, estimated-$S$, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:
- Volatilization: based on calculated Henry’s law constant, the estimated $t_\frac{1}{2} \approx 9.9$ d from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).
- Photooxidation:
- Hydrolysis:
- Biodegradation: average rate of biodegradation 41.0 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).
- Biotransformation:
- Bioconcentration Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environmental Compartments:
- Air: estimated photooxidation $t_\frac{1}{2} \approx 0.44$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1993).
- Surface water:
- Ground water:
- Sediment:
- Soil:
- Biota:

### TABLE 12.1.1.6.1
Reported aqueous solubilities of furfural (2-furaldehyde) at various temperatures

<table>
<thead>
<tr>
<th>Temperature /°C</th>
<th>Solubility S/g·m$^{-3}$</th>
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<td>147400</td>
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</table>
Aldehydes and Ketones

FIGURE 12.1.1.6.1 Logarithm of mole fraction solubility (ln \( x \)) versus reciprocal temperature for furfural.

TABLE 12.1.1.6.2
Reported vapor pressures of furfural (2-furaldehyde) at various temperatures and the coefficients for the vapor pressure equations

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

Evans & Aylesworth 1926

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>Stull 1947</th>
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<th>Matthews et al. 1950</th>
<th>Ramsay-Young method</th>
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<th>t/°C</th>
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<th>mp/°C</th>
<th>∆HV/(kJ mol⁻¹) = 38.59 at bp</th>
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<tr>
<td>161.8</td>
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(Continued)
### TABLE 12.1.1.6.2 (Continued)

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<td><strong>ebulliometry</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>Ramsay-Young method</strong></td>
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<td>P/Pa</td>
<td>t/°C</td>
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**FIGURE 12.1.1.6.2** Logarithm of vapor pressure versus reciprocal temperature for furfural.
Benzaldehyde

Common Name: Benzaldehyde
Synonym: benzenecarbonal, oil of bitter almonds
Chemical Name: benzaldehyde
CAS Registry No: 100-52-7
Molecular Formula: C₇H₆O, C₆H₅CHO
Molecular Weight: 106.122
Melting Point (°C):
−57.1 (Lide 2003)
Boiling Point (°C):
178.8 (Lide 2003)
Density (g/cm³ at 20°C):
1.0401 (24.94°C, measured, Ambrose et al. 1975)
1.0447 (Dean 1985)
1.0446 (Riddick et al. 1986)
Molar Volume (cm³/mol):
102.0 (calculated-density, Chiou 1985)
118.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion $\Delta H_{fus}$ (kJ/mol):
9.322 (Riddick et al. 1986)
Entergy 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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2991 (quoted, Deno & Berkheimer 1960)
2857 (1 in 350 parts, Merck Index 1960)
3490, 3500 (quoted Ph. D. theses from University of London, Mitchell et al. 1964)
6550, 6580 (shake flask-gravimetric method, shake flask-GC/FID, Mitchell et al. 1964)
6900–7000 (shake flask-refractive index method, Carlless & Swarbrick 1964)
7200 (20°C, shake flask-GC, Tewari et al. 1982)
3000 (20–25°C, shake flask-GC, Urano et al. 1982)
3300 (Verschueren 1983)
3279 (shake flask-GC, Chiou 1985)
3000 (20°C, Riddick et al. 1986)
7200*, 7400 (20°C, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993)
3514 (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):
133.3*, 145.2 (26.2°C, extrapolated-regression of tabulated data, temp range 26.2–179°C, Stull 1947)
log (P/mmHg) = [−0.2185 × 11657.8/(T/K)] + 8.580362; temp range 26.2–179°C (Antoine eq., Weast 1972–73)
137.0* (ebulliometry-extrapolated from Antoine eq., measured range 38.5–89.3°C, Ambrose et al. 1975b)
log (P/kPa) = 6.20251 – 161.1217/(T/K – 67.984); temp range 38.5–89.3°C, mercury as reference, Ambrose et al. 1975b)
log (P/kPa) = 6.22556 – 1628.007/(T/K – 66.119); temp range 74.9–190.8°C, water as reference, Ambrose et al. 1975b)
169.0 (calculated from different vapor eq., Ambrose et al. 1975)
160.5 (extrapolated-Antoine eq., Ambrose et al. 1979)
133.3 (26.0°C, Verschueren 1983)
160.5 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.21282 – 1618.669/(205.994 + t°C); temp range 38.5–208°C (Antoine eq. from reported exp. data of Ambrose et al. 1975, Boublík et al. 1984)
169.0 (Riddick et al. 1986)
log (P_2/kPa) = 5.56823 – 1197.54/(–115.829 + T/K); temp range 348–452 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_3/kPa) = 7.4764 – 2455.4/(T/K); temp range 273–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_4/kPa) = 6.20256 – 1611.255/(–67.979 + T/K); temp range 409–481 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_5/kPa) = 6.48764 – 1782.204/(–52.863 + T/K); temp range 311–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/L/kPa) = 6.22745 – 1629.229/(–65.993 + T/K); temp range 370–475 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P/mmHg) = 28.4711 – 3.4489 × 10^3/( T / K )–6.8363 · log( T / K )–2.8173×10–10·(T/K) + 9.5236 × 10–7·(T/K)^2; temp range 247–695 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. Additional data at other temperatures designated * are compiled at the end of this section):
2.781, 1.494 (quoted exp.), calculated-bond contribution, Hine & Mookerjee 1975)
2.815 (Gaffney et al. 1987)
2.71* (gas stripping-GC, measured range 15–45°C, Betterton & Hoffmann 1988)
ln [K_H/W/(M/atm)] = –5.00 + 1977/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
ln [K_H/W/(M/atm)] = –5.90 + 2207/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1), Zhou & Mopper 1990)
3.08* (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)
ln K_AW = –6759/(T/K) + 15.93 (EPICS-UV, temp range 5–25°C, Allen et al. 1998)
1.94* (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_AW = 4.665 – 2275/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.48 (Leo et al. 1971; Hansch et al. 1972)
1.45 (shake flask-UV at pH 5.62, Umeayama et al. 1971)
1.43 (shake flask-UV, Holmes & Lough 1976)
1.45 ± 0.03 (shake flask at pH 7, Unger et al. 1978)
2.33 (HPLC-RT correlation, Veith et al. 1979)
1.56 (HPLC-k’ correlation, Eadsforth 1986)
1.49 (shake flask, Eadsforth 1986)
1.44 (HPLC-RT correlation average, Ge et al. 1987)
1.54 (RP-HPLC-RT correlation, ODS column with masking agent, Bechaly et al. 1989)
1.48 (recommended, Sangster 1989, 1993)
1.72 (shake flask-UV, Kramer & Henze 1990)
1.48 (shake flask-UV spec., Alcron et al. 1993)
1.48 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization:
Photolysis: loss rate k = 3.4 × 10^{-4} min^{-1} in outdoor Teflon chambers in dark (Grosjean 1985).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:
k < 2.0 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen in the aquatic systems at 25°C with t_{1/2} > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
k_{OH} = 1.3 \times 10^{-11} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) determined by the long-path Fourier transform IR spectroscopic method with reference to that for C_2H_4 or C_2D_4 (Niki et al. 1978)

k_{OH} = 7.6 \times 10^9 \text{ M}^{-1}\text{ s}^{-1}\) at 25°C with t_{1/2} = 0.74 d (Hendry & Kenley 1979; quoted, Mill 1982)

k_{OH} = 7.8 \times 10^{12} \text{ cm}^3\text{ mol}^{-1}\text{ s}^{-1}\) at 300 K (Lyman 1982)

k = (2.5 \pm 0.5) \text{ M}^{-1}\text{ s}^{-1}\) for 2-10 mM to react with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)

k_{NO_3} = < 9.6 \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) at 300 ± 1 K (using relative rate technique to propene Carter et al. 1981; quoted, Atkinson 1991)

k_{NO_3} = (2.55 \pm 0.08) \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) at 294 K (Atkinson et al. 1984; quoted, Atkinson 1991)

k_{NO_3} = (1.13 \pm 0.25) \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\), compared to a previous measured value k_{NO_3} < 5.2 \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) (relative rate technique, Atkinson et al. 1984)

k_{OH} = 2.0 \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

k_{NO_3} = 1.30 \times 10^{-11} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\), k_{OH}(calc) = 1.698 \times 10^{-11} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) (SAR, Atkinson 1987, 1990; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

k_{NO_3} = (2.54 \times 10^{-15} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

k_{OH} = 1.29 \times 10^{-11} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 11.40 \times 10^{-12} \text{ cm}^3\text{-molecule}^{-1}\text{ s}^{-1}\) (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation 119.0 mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976), biodegradation rate constant k = 0.065–0.074 h⁻¹ in 30 mg/L activated sludge after a lag time of 5–10 h (Urano & Kato 1986b).

Biotransformation:

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

Half-Lives in the Environment:

Air: t_{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 hydroxyl radical (Darnall et al. 1976); t_{1/2} = 0.74 d based on rate constants for oxidation by OH radical in the atmosphere at 25°C (Mill 1982); loss rate k = (3.4 \pm 1.7) \times 10^{-4} \text{ min}^{-1}\) in outdoor Teflon chambers in the dark (Grosjean 1985); calculated lifetimes of 11 h and 18 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

### TABLE 12.1.1.7.1
Reported aqueous solubilities of benzaldehyde at various temperatures

<table>
<thead>
<tr>
<th>Stephenson 1993</th>
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<td>80.0</td>
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FIGURE 12.1.1.7.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.2
Reported vapor pressures of benzaldehyde at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Ambrose et al. 1975b</th>
</tr>
</thead>
<tbody>
<tr>
<td>summary of literature data</td>
<td>comparative ebulliometry</td>
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</table>

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

| at 25°C | at bp |
| 50.3 | 42.6 |

\(\rho/kg m^{-3}\)

\(\text{Antoine eq.}\)

| eq. 3 | \(P/kPa\) | \(167.121\) | \(74923\) | 148.806 | 44737 |

\(\text{Antoine eq.}\)

| \(P/kPa\) | 148.806 | 44737 | 292.94 | 1044.85 |
| 155.366 | 54140 | 298.09 | 1040.13 |

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TABLE 12.1.1.7.2 (Continued)

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Antoine eq.

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FIGURE 12.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for benzaldehyde.
TABLE 12.1.1.7.3
Reported Henry’s law constants of benzaldehyde at various temperatures and temperature dependence equations

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

Zhou & Mopper 1990

gas stripping-HPLC/UV

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<th>t/°C</th>
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<tr>
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<td>-</td>
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eq. 1a

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</table>

Zhou & Mopper 1990

gas stripping-HPLC/UV

Betterton & Hoffmann 1988

gas stripping-GC, spec.

Allen et al. 1998

EPICS-UV

\[\Delta H/(kJ \text{ mol}^{-1}) = -42.2\text{ at }25°C\]

\[\Delta S/(J \text{ K}^{-1} \text{ mol}^{-1}) = 132.4\]

FIGURE 12.1.1.7.3 Logarithm of Henry’s law constant versus reciprocal temperature for benzaldehyde.
12.1.2 KE TONES

12.1.2.1 Acetone

![Acetone molecule]

Common Name: Acetone
Synonym: 2-propanone, dimethylketone, DMK
Chemical Name: acetone, 2-propanone
CAS Registry No: 67-64-1
Molecular Formula: C₃H₆O, CH₃COCH₃
Molecular Weight: 58.079

Melting Point (°C):
-94.7  (Lide 2003)

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

Density (g/cm³ at 20°C):
0.7899  (Weast 1982–83)
0.7908  (Dean 1985)

Molar Volume (cm³/mol):
73.5  (20°C, calculated-density)
74.0  (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion \(\Delta H_{\text{fus}}\) (kJ/mol):
5.690  (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/m³ or mg/L at 25°C or as indicated):
miscible  (20°C, Palit 1947)
miscible  (Dean 1985; Yaws et al. 1990)
miscible  (Riddick et al. 1986; Howard 1990)
217700, 453000 (pseudo-solubilities, Staples 2000)

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

29610*  (interpolated-regression of tabulated data, temp range –59.4 to 56.5°C, Stull 1947)

\[
\log (P/\text{mmHg}) = 7.19038 - 1233.4/(230 + t/°C) \quad \text{(Antoine eq., Dreisbach & Martin 1949)}
\]

30490  (Perry 1950)

51854*  (37.68°C, temp range 37.68–56.02°C, Brown & Smith 1957)

30800  (Buttery et al. 1969)

30810  (Hoy 1970)


\[
\log (P/\text{mmHg}) = -0.2185 \times 10577.7/(T/K) + 9.143231; \text{temp range –20 to 96°C} \quad \text{(Antoine eq., Weast 1972–73)}
\]

30780, 30800 (calculated-Antoine eq., Boublík et al. 1973)

\[
\log (P/\text{mmHg}) = 7.15853 - 1231.232/(231.766 + t/°C); \text{temp range 37.6–56.02°C} \quad \text{(Antoine eq. from reported exptl. data, Boublik et al. 1973)}
\]

\[
\log (P/\text{mmHg}) = 7.11714 - 1210.595/(229.664 + t/°C), \text{temp range 37.6–56.02°C} \quad \text{(Antoine eq. from reported exptl. data, Boublík et al. 1973)}
\]

30810*  (ebulliometry, fitted to Antoine eq., measured range 259–350.9 K, Ambrose et al. 1974)

\[
\log (P/\text{kPa}) = 6.25632 - 1217.904/(T/K - 42.692); \text{temp range 311.7–350.9 K, or for pressure range 53–202 kPa} \quad \text{(Antoine eq., ebulliometry, Ambrose et al. 1975a)}
\]

\[
\log (P/\text{kPa}) = 6.25478 - 1216.689/(T/K - 42.875); \text{temp range 259.17–350.9 K, or for pressure below 225 kPa} \quad \text{(Antoine eq., ebulliometry, Ambrose et al. 1974)}
\]

30870, 31520 (quoted exptl., calculated-Antoine eq., Boublík et al. 1984)
log \( \log (P/kPa) = 6.24039 - 1209.746/(229.574 + t/°C) \); temp range –12.95 to 55.3°C (Antoine eq. from reported
exptl. data, Boublik et al. 1984)
log \( \log (P/kPa) = 6.26017 - 1214.208/(230.002 + t/°C) \); temp range –13.98 to 77.72°C (Antoine eq. from reported
exptl. data of Ambrose et al. 1974, Boublik et al. 1984)
log \( \log (P/kPa) = 6.28185 - 1230.342/(231.665 + t/°C) \); temp range 37.6–56.02°C (Antoine eq. from reported exptl.
data of Brown & Smith 1957, Boublik et al. 1984)
30780 (calculated-Antoine eq., Dean 1985)
log \( \log (P/mmHg) = 7.11714 - 1210.595/(229.664 + t/°C) \), temp range: liquid (Antoine eq., Dean 1985, 1992)
24227, 30806 (20, 25°C, Riddick et al. 1986)
log \( \log (P/kPa) = 6.25478 - 1216.589/(230.275 + t/°C) \), temp range not specified (Antoine eq., Riddick et al. 1986)
30730 (interpolated-Antoine eq.-V, Stephenson & Malanowski 1987)
log \( \log (PL/kPa) = 6.24204 - 1210.6/(–43.49 + T/K) \); temp range 261–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \( \log (PL/kPa) = 6.75622 - 1566.69/(0.269 + T/K) \); temp range 329–488 K (Antoine eq.-II, Stephenson &
Malanowski 1987)
log \( \log (PL/kPa) = 3.6452 – 469.5/(–108.21 + T/K) \); temp range 178–243 K (Antoine eq.-III, Stephenson &
Malanowski 1987)
log \( \log (PL/kPa) = 6.19735 – 1190.382/(–45.373 + T/K) \); temp range 203–269 K (Antoine eq.-IV, Stephenson &
Malanowski 1987)
log \( \log (P/\text{mmHg}) = 28.5884 – 2.469 \times 10^3/(T/K) – 7.351\cdot\log (T/K) + 2.8025 \times 10^{-10}\cdot(T/K) + 2.7361 \times 10^{-6}\cdot(T/K)^2 \); temp
range 178–508 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section):
3.34 (partial pressure, Butler & Ramchandani 1935)
3.96 (shake flask, partial vapor pressure-GC, Burnett 1963)
3.25 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
3.97 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
4.02, 3.93, 2.91 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
4.05 (headspace-GC, Vitenberg et al. 1975)
4.10 (calculated-activity coeff and vapor pressure, γP, Rathbun & Tai 1982)
0.908, 3.93 (0, 25°C, headspace-GC, Snider & Dawson 1985)
3.38 (review, Gaffney et al. 1987)
2.928* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
ln \[ \log \left( \frac{K_{H}}{\text{M/atm}} \right) = –5.00 + 1977/(T/K) \]; temp range 10–45°C (gas stripping-HPLC measurements, freshwater,
Zhou & Mopper 1990)
ln \[ \log \left( \frac{K_{H}}{\text{M/atm}} \right) = –3.60 + 1518/(T/K) \]; temp range 25–45°C (gas stripping-HPLC measurements, seawater
(salinity 35 ± 1), Zhou & Mopper 1990)
3.07* (gas stripping-GC, measured range –14.9 to 44.9°C, Betterton 1991)
4.33 (computed, Yaws et al. 1991)
0.722, 1.26, 2.045, 5.31, 7.514 (0.51, 9.0, 16.11, 31, 38.51°C, headspace-GC, de-ionized water, Benkelberg et al. 1995)
3.735* (headspace-GC, rain water, measured range –30 to 39.51°C, Benkelberg et al. 1995)
0.762, 2.19, 6.64, 10.30 (0, 14.51, 30, 39.51°C, headspace-GC, artificial seawater, Benkelberg et al. 1995)
ln \[ \log \left( \frac{k_{H}}{\text{atm}} \right) = (18.4 ± 0.3) – (5386 ± 100)/(T/K) \]; temp range 10–40°C (headspace-GC measurements, Benkelberg
et al. 1995)
2.56 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
9.92 (EPICS-GC, Ayuttaya et al. 2001)
2.58 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log \( K_{AW} = 3.742 – 1965/(T/K) \) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log $K_{OW}$:
-0.24 (shake flask-CR, Collander 1951)
-0.24 (shake flask at pH 7, Unger et al. 1978)
-0.48 (shake flask-GC, Tanii et al. 1986)
-0.24 (recommended, Sangster 1989, 1993)
-0.31 (CPC centrifugal partition chromatography, Gluck & Martin 1990)
-0.37 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
-0.24 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
-0.187 (calculated, Staples 2000)

Sorption Partition Coefficient, log $K_{OC}$:
-0.586 (calculated-$K_{OW}$, Kollig 1993)
-0.523 (quoted calculated value, Staples 2000)

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

Volatilization: using Henry’s law constant, $t_\frac{1}{2} = 20$ 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: rate constant $k = 1.4 \times 10^{-5}$ s$^{-1}$ in the atmosphere (Carlier et al. 1986); calculated lifetime $\tau \sim 60$ d in air (Atkinson 2000)

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

photooxidation $t_\frac{1}{2} = 11.3$–453 yr, based on measured data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_\frac{1}{2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = (0.23 \pm 0.03) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k_{OH} = (0.62 \pm 0.09) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (relative rate technique to n-hexane, Chiorboli et al. 1983; quoted, Atkinson 1985)

$k = 0.032 \pm 0.006$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2 and 20–23°C (Hoiné & Bader 1983)

$k_{OH}$(calc) = $2.2 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}$(obs.) = 2.3 $\times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_\frac{1}{2} = 279$–2790 h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{OH} = 2.16 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K and $k = 1.80 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the aqueous-phase reaction with hydroxyl radical in solution (Wallington & Kurylo 1987)

$k_{OH} = 2.16 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k$(soln) = 1.8 $\times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = 2.26 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}$(calc) = 0.18 $\times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: biodegradation rate constants, $k = 0.016$–0.020 h$^{-1}$ in 30 mg/L activated sludge after a time lag of 20–25 h (Urano & Kato 1986b);

$t_\frac{1}{2}$(aq. aerobic) = 24–168 h, based on unacclimated aqueous screening test data (Bridie et al. 1979; Dore et al. 1975; selected, Howard et al. 1991);

t$_{aq.}$(anaerobic) = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$k(\text{exptl}) = 0.0440 \, h^{-1}$ compared to predicted rate constants by group contribution method: $k = 0.0433 \, h^{-1}$ (nonlinear) and $k = 0.043 \, h^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_\alpha > 9.9$ 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 $t_\alpha = 279–2790$ h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

calculated lifetimes $\tau = 53$ d and $\tau > 11$ yr for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000);

photooxidation and photolysis $t_\alpha = 36$ h (Staples 2000).

Surface water: photooxidation $t_\alpha = 11.3–453$ yr, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991);

t$\alpha = 24–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aerobic biodegradation $t_\alpha = 96–168$ h (Staples 2000).

Ground water: $t_\alpha = 48–336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_\alpha = 384$ h or 16 d (Staples 2000).

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

aerobic biodegradation $t_\alpha = 96–168$ h (Staples 2000).

Biota:

**TABLE 12.1.2.1.1**

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

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<table>
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equation for vapor pressures below 200 kPa

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

at 25°C 31.3

at bp 29.6
**FIGURE 12.1.2.1.1** Logarithm of vapor pressure versus reciprocal temperature for acetone.

**TABLE 12.1.2.1.2**
Reported Henry's law constants of acetone at various temperatures and temperature dependence equations

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

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2.

Benkelberg et al. 1995

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Artificial sea water

For deionized and rain water: 14.51 2.189

Eq. 3

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FIGURE 12.1.2.1.2 Logarithm of Henry’s law constant versus reciprocal temperature for acetone.
12.1.2.2 2-Butanone (Methyl ethyl ketone)

Common Name: Methyl ethyl ketone
Synonym: 2-butanone, butan-2-one, MEK
Chemical Name: 2-butanone, methyl ethyl ketone
CAS Registry No: 78-93-3
Molecular Formula: C₄H₈O, CH₃CH₂COCH₃
Molecular Weight: 72.106
Melting Point (°C):
−86.64 (Lide 2003)
Boiling Point (°C):
79.59  (Lide 2003)
Density (g/cm³ at 20°C):
0.8054 (Weast 1982–83)
0.7997 (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
89.9 (calculated-density, Rohrschneider 1973)
96.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
14.7 (pKₐ, Riddick et al. 1986)
−7.2 (pKₐH⁺, Riddick et al. 1986)
Enthalpy of Fusion ∆H₉₄ (kJ/mol):
8.439 (Riddick et al. 1986)
Entropy of Fusion ∆S₉₄ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S₉₄ = 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):
240000 (20°C, synthetic method, Jones 1929; quoted, Palit 1947; Dean 1985; Riddick et al. 1986)
255700* (shake flask-volumetric method, measured range 20–30°C Ginnings et al. 1940)
343550 (shake flask-volumetric, Ginnings et al. 1940)
228020 (estimated, McGowan 1954)
12420 (20°C, Amidon et al. 1975)
136280 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
353000 (20°C, Verschueren 1983)
249000 (selected, Yaws et al. 1990)
276000*, 235000 (19.3°C, 29.7°C, shake flask-GC, measured range 0–70.2°C, Stephenson 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):
12954* (interpolated-regression of tabulated data, temp range −48.3 to 79.6°C, Stull 1947)
log (P/mmHg) = 7.22200 − 1343.6/(230 + t/°C), (Antoine eq., Dreisbach & Martin 1949)
16500* (31.84°C, ebulliometry, measured range 31.84–79.5°C, Dreisbach & Shrader 1949)
25158* (41.46°C, flow calorimetry, measured range 41.46–79.5°C, Nickerson et al. 1961)
26568* (42.77°C, ebulliometry, measured range 42.778–88.44°C, Collerson et al. 1965)
log (P/mmHg) = 7.06376 − 1261.455/(221.982 + t/°C); temp range 42.778–88.444°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = 19.48322 − 2328.0/(T/K) − 3.92657·log (T/K); temp range 42.778–88.444°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = [−0.2185 × 8149.5/(T/K)] + 7.959295; temp range −48.3 to 79.6°C (Antoine eq., Weast 1972–73)
Aldehydes and Ketones

12079* (ebulliometry, Ambrose et al. 1975a; quoted, Riddick et al. 1986; Howard 1990)
12000, 12060, 12640 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.02273 – 1167.861/(211.199 + t/°C); temp range 41.46–97.42°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.18397 – 1258.948/(221.725 + t/°C); temp range 42.78–86.44°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
log (P/kPa) = 6.18838 – 1261.297/(222.964 + t/°C); temp range 42.79–88.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
12020 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.06356 – 1261.34/(221.97 + t/°C); temp range 43–88°C (Antoine eq., Dean 1985, 1992)
12700 (Howard et al. 1986; quoted, Banerjee et al. 1990)
12120 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.24715 – 1294.53/(–47.442 + T/K); temp range 294–352 K (Antoine eq-I., Stephenson & Malanowski 1987)
log (PL/kPa) = 6.18479 – 1259.519/(–51.359 + T/K); temp range 315–363 K (Antoine eq-II., Stephenson & Malanowski 1987)
log (PL/kPa) = 6.22518 – 1286.794/(–47.766 + T/K); temp range 353–403 K (Antoine eq-III., Stephenson & Malanowski 1987)
5425 (calculated-solvatochromic parameters, Banerjee et al. 1990)
log (P/mmHg) = 47.706 – 3.0965 × 10³/(T/K) – 15.184·log (T/K) + 7.4846 × 10–3·(T/K) – 1.7084 × 10–13·(T/K)²; temp range 186–536 K (vapor pressure eq., Yaws 1994)
12071* (static method-manometry, measured range 0–50°C, Garriga et al. 1996)

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):
4.710 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
4.723 (quoted, exptl., Hine & Mookerjee 1975)
5.549, 4.408 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
3.87 (headspace-GC, Vitenberg et al. 1975)
0.987, 5.76 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
ln [H/(atm·m³/mol)] = –26.32 – 5214/(T/K), temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)
5.210 (gas stripping-HPLC/UV, Zhou & Mopper 1990)
5.117* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
ln [KH/(M/atm)] = –6.03 + 2184/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
ln [KH/(M/atm)] = –5.97 + 2138/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1 l), Zhou & Mopper 1990)
18.28* (45°C, equilibrium headspace-GC, measured range 45–80°C, Ettre et al. 1993)
3.85 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
3.95 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log KAW = 4.764 – 2213/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
5.04 – 3.54 (27°C, equilibrium headspace-GC, solute concn 10.01–85.10 mg/L, measured range 300–315 K, Cheng et al. 2003)

Octanol/Water Partition Coefficient, log Kow:
0.26 (shake flask-CR, Collander 1957)
0.28 (shake flask-UV, Fujita et al. 1964, Hansch & Leo 1979)
0.32 ± 0.01 (shake flask-UV, calculated, Iwasa et al. 1965)
0.29 (shake flask-UV, GC, Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1969, 1971)
0.28 ± 0.02 (shake flask at pH 7, Unger et al. 1978)
Octanol/Air Partition Coefficient, log $K_{OA}$:

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

Bioconcentration Factor, log BCF:

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

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

1.53 (soil, estimated-$K_{OW}$, Lyman et al. 1982; quoted, Howard 1990)
1.47 ± 0.55, 1.53 ± 0.88, 1.50 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
0.070 (predicted-$K_{OW}$, Walton et al. 1992)
–0.03 (calculated-$K_{OW}$, Kollig 1993)

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

Volatilization: based on lab. data for evaporation relative to the reaeration rate of 0.27 (Mackay et al. 1982; Rathbun & Tai 1982; quoted, Howard 1990) and typical reaeration rates of rivers and lakes (Mill et al. 1982; quoted, Howard 1990), $t_{1/2} = 3$ d for evaporation from a river and $t_{1/2} = 12$ d from lake (Howard 1990).

Photolysis: rate constant $k = 1.4 \times 10^{-5}$ s$^{-1}$ in the atmosphere (Carlier et al. 1986); calculated lifetime $\tau \sim 4$ d in air (Atkinson 2000)

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

photooxidation $t_{1/2} = 48.8 – 81.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; selected, Howard et al. 1991)
photooxidation $t_{1/2} = 2.4 – 24$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976)

$k_{OH} = (0.20 \pm 0.06) \times 10^{10}$ cm$^3$ M$^{-1}$ s$^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

$k < 2.0 \times 10^2$ M$^{-1}$ s$^{-1}$ for oxidation with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 0$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 1.9 \times 10^9$ M$^{-1}$ s$^{-1}$ at 25°C with $t_{1/2} = 2.9$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (0.95 \pm 0.09) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at (295 ± 2) K in air (relative rate technique to ethene Cox et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (1.20 \pm 0.20) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K in air (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k = (0.12 \pm 0.02)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water using 20–300 mM $t$-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH(calc)} = 1.38 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH(obs.)} = 1.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.97 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 24°C with an atmospheric lifetime $\tau = 12$ d (Edney et al. 1986)

$k_{OH} = 1.15 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K and $k$(soln) = $1.50 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{OH} = 1.15 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

photooxidation $t_{1/2} = 64.2 – 642$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Howard et al. 1991)

$k_{OH(calc)} = 1.65 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: first-order hydrolysis $t_{1/2} > 0$ yr, based on nonreactive hydrolysis from pH 5 to 9 at 15°C (Kollig et al. 1987; selected, Howard et al. 1991).
Biodegradation:

- \( k = 0.021 - 0.025 \text{ h}^{-1} \) in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b)
- \( t_{1/2}^{(aq. \text{ aerobic})} = 24 - 168 \text{ h} \), based on unacclimated grab sample of aerobic freshwater (Dojilido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)
- \( t_{1/2}^{(aq. \text{ anaerobic})} = 96 - 672 \text{ h} \), based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
- \( t_{1/2}^{(aerobic)} = 1 \text{ d} \), \( t_{1/2}^{(anaerobic)} = 28 \text{ d} \) in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: \( t_{1/2} = 2.4 - 24 \text{ h} \) in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
- Photodecomposition \( t_{1/2} = 9.8 \text{ h} \) under simulated atmospheric conditions, with NO (Dilling et al. 1976)
- \( t_{1/2} = 2.3 \text{ d} \) for the atmospheric reaction with photochemically produced hydroxyl radical (Cox et al. 1981; quoted, Howard 1990);
- Photooxidation \( t_{1/2} = 64.2 - 642 \text{ h} \), based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);
- Calculated atmospheric lifetime \( \tau = 12 \text{ d} \) due to reaction with OH radical (Edney et al. 1986) atmospheric transformation lifetime \( \tau < 1 \text{ d} \) (estimated, Kelly et al. 1994);
- Calculated lifetime \( \tau = 10 \text{ d} \) for reaction with OH radical (Atkinson 2000).

Surface water:
- Photooxidation \( t_{1/2} = 48.8 - 81.4 \text{ yr} \), based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; quoted, Howard et al. 1991); \( t_{1/2} = 24 - 168 \text{ h} \), based on unacclimated grab sample of aerobic freshwater (Dojilido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)
- \( t_{1/2}^{(aerobic)} = 1 \text{ d} \), \( t_{1/2}^{(anaerobic)} = 28 \text{ d} \) in natural waters (Capel & Larson 1995).

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

Sediment:

Soil: calculated \( t_{1/2} = 4.9 \text{ d} \) from first-order kinetic of degradation under both sterile and nonsterile conditions (Anderson et al. 1991);
- \( t_{1/2} = 24 - 168 \text{ h} \), based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

### TABLE 12.1.2.2.1

Reported aqueous solubilities of 2-butanone (methyl ethyl ketone) at various temperatures

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2-Butanone (methyl ethyl ketone): solubility vs. 1/T

FIGURE 12.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.2
Reported vapor pressures of 2-butanone (methyl ethyl ketone) at various temperatures and the coefficients for the vapor pressure equations

- log P = A – B/(T/K) (1)
- ln P = A – B/(T/K) (1a)
- log P = A – B/(C + t/°C) (2)
- ln P = A – B/(C + t/°C) (2a)
- log P = A – B/(C + T/K) (3)
- ln P = A – B/(C + T/K) (3a)
- log P = A – B/(T/K) – C·log (T/K) (4)

1.

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Stull 1947

Dreisbach & Shrader 1949

Nickerson et al. 1961

Collerson et al. 1965

Summary of literature data

ebulliometry

flow calorimetry

ebulliometry

A 21.78963

B 2441.9

C 4.70504

mp/°C 86.69

bp/°C 79.589
### TABLE 12.1.2.2.2 (Continued)

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<td>Kirchhoff eq.</td>
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**∆HV/(kJ mol⁻¹) = 31.67**

#### 2.

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<td>P/Pa</td>
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<td>eq. 3a P/kPa</td>
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<td>C</td>
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</table>

**bp/°C | 79.583**
**eq. 2 P/kPa | 6.18444**
**A | 1259.223**
**B | –51.392**

**∆HV/(kJ mol⁻¹) =**
- at 25°C | 34.7
- at bp | 31.8
FIGURE 12.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.3
Reported Henry's law constants of 2-butanone (methyl ethyl ketone) at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{aw} &= A - B/(T/K) \quad (1) \\
\ln (1/K_{aw}) &= A - B/(T/K) \quad (2) \\
\ln [H/(Pa \cdot m^3/mol)] &= A - B/(T/K) \quad (4) \\
K_{aw} &= A - B\cdot(T/K) + C\cdot(T/K)^2 \quad (5)
\end{align*}
\]

Snider & Dawson 1985  
Ashworth et al. 1988  
Zhou & Mopper 1990

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<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
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<th>H/(Pa m³/mol)</th>
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<td>25</td>
<td>6.666</td>
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<td>∆H/(kJ mol⁻¹) = 46.024</td>
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<tr>
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<td>-</td>
<td>40</td>
<td>14.07</td>
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<tr>
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<td>H/(atm m³/mol)</td>
<td>eq. 1a</td>
<td>K_{aw}′/(M/atm)</td>
<td>eq. 1a</td>
<td>K_{aw}′/(M/atm)</td>
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<tr>
<td></td>
<td>A = -26.32</td>
<td>B = -5214</td>
<td>A = -6.03</td>
<td>B = -2184</td>
<td>B = -2138</td>
</tr>
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</table>
FIGURE 12.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-butanone.
12.1.2.3 2-Pentanone

Common Name: 2-Pentanone
Synonym: 2-pentanone, methyl propyl ketone, methyl \( n \)-propyl ketone, ethylacetone
Chemical Name: 2-pentanone, methyl propyl ketone
CAS Registry No: 107-87-9
Molecular Formula: \( \text{C}_5\text{H}_{10}\text{O}, \text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_3 \)
Molecular Weight: 86.132
Melting Point (°C):
-77.80 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1990)
-76.8 (Lide 2003)
Boiling Point (°C):
102.0 (Weast 1982–83; Verschueren 1983)
101.7 (Dean 1985; Howard 1990)
102.26 (Lide 2003)
Density (g/cm³ at 20°C):
0.8089 (Weast 1982–83)
0.8064, 0.8015 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
118.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion \( \Delta H_{\text{fus}} \) (kJ/mol):
2.541 (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/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
54268* (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)
30150 (30°C, Gross et al. 1939)
55100 (shake flask-volumetric, Ginnings et al. 1940)
59500 (20°C, shake flask-volumetric, Ginnings et al. 1940)
64010 (shake flask-interferometer, Donahue & Bartell 1952)
54350 (McGowan 1954; Deno & Berkheimer 1960)
43000 (Verschueren 1977, 1983)
59500 (20°C, Riddick et al. 1986)
55400 (selected, Yaws et al. 1990)
59000* (19.7°C, shake flask-GC, measured range 0–90.5°C, Stephenson 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2088* (interpolated-regression of tabulated data, temp range –12.7 to 102.7°C, Stull 1947)
2666 (28.5°C, Stull 1947)
20440* (56.649°C, ebulliometry, measured range 56.5–111.655°C, Collerson et al. 1965)
\[ \log (P/\text{mmHg}) = 7.01753 – 1311.145/(214.693 + t/°C); \text{temp range 56.5–111.65°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)} \]
\[ \log (P/\text{mmHg}) = 21.71880 – 2694.12/(T/K) – 4.63307 \log (t/°C); \text{temp range 56.5–111.65°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)} \]
\[ \log (P/\text{mmHg}) = 6.13916 – 1379.06/(221.41 + t/°C); \text{temp range –5 to 100°C (data fitted to Antoine eq., static method-Ramsey-Young apparatus measurements, Meyer & Wagner 1966)} \]
\[ \log (P/\text{mmHg}) = [-0.2185 \times 11240.6/(T/K)] + 9.432089; \text{temp range –12–103.3°C (Antoine eq., Weast 1972–73)} \]
4720* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
2133 (quoted, Verschueren 1983)
Aldehydes and Ketones

1621 (quoted, Mackay & Yuen 1983)
4648 (extrapolated-Antoine eq., Boublik et al. 1984)

\[ \log (P/kPa) = 6.14908 - 1311.372/(214.222 + t/°C), \text{ temp range } 61.72-121.4°C \]  
(Antoine eq. from reported exptl. data, Boublik et al. 1984)

\[ \log (P/mmHg) = 7.02193 - 1313.85/(215.01 + t/°C), \text{ temp range } 56-111°C \]  
(Antoine eq., Dean 1985, 1992)

4702 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P/kPa) = 6.14243 - 1311.145/(-58.457 + T/K), \text{ temp range } 329-386 K \]  
(Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log (P/kPa) = 6.1404 - 1310.269/(-58.514 + T/K), \text{ temp range } 336-422 K \]  
(Antoine eq.-II, Stephenson & Malanowski 1987)

\[ \log (P/kPa) = 6.47975 - 1569.596/(-24.035 + T/K), \text{ temp range } 416-501 K \]  
(Antoine eq.-III, Stephenson & Malanowski 1987)

\[ \log (P/mmHg) = 18.3056 - 2.3477 \times 10^3/(T/K) - 3.6667\cdot\log (T/K) + 7.1502 \times 10^{-4}\cdot(T/K) + 1.0912 \times 10^{-13}\cdot(T/K)^2; \]  
(temp range 196–561 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
10.91 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
6.44 (partial vapor pressure-GC, Buttery et al. 1969)
6.52 (quoted, exptrl., Hine & Mookerjee 1975)
7.66, 6.52 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
3.83 (calculated-γP, Rathbun & Tai 1982)
5.876 (gas-stripping, Hawthorne 1984)
10.13 (modified gas-stripping, Hawthorne et al. 1985)
8.47, 6.83 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
0.91 ± 0.03 (shake flask-UV at pH 7, Unger et al. 1978)
0.91 (Hansch & Leo 1985)
0.78 (shake flask-GC, Tani et al. 1986)
0.87 (calculated-\( V_i \) and solvatochromic parameters, Kamlet et al. 1988)
0.95 (calculated-activity coeff. \( \gamma \) from UNIFAC, Banerjee & Howard 1988)
0.84 (recommended, Sangster 1989; 1993)
0.91 (recommended, Hansch et al. 1995)

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

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

Sorption Partition Coefficient, log \( K_{oc} \):
1.869 (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, \( t_{1/2} = 15.5 \) h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and \( t_{1/2} = 14.5 \) h in a wind-wave tank with a 6 m/s wind speed (Howard 1990).

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 \( k_03 \) with O\(_3\) or as indicated, *data at other temperatures see reference:

\[ k_{OH} = (4.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at (299 ± 2) K (relative rate technique to cyclohexane Atkinson et al. 1982; quoted, Atkinson 1985)

\[ k \sim 0.02 \text{ M}^{-1} \text{ s}^{-1} \] for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
k_{OH}(calc) = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{OH}(obs.) = 4.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)}

k_{OH} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K and } k(\text{soln}) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)}

k_{OH} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)}

k_{OH}(calc) = 5.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1996)}

k_{OH} = (4.56 \pm 0.30) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 2 \text{ K with calculated tropospheric lifetime } \tau = 2.5 \text{ d (relative rate method, Atkinson et al. 2000)}

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: \( t_{1/2} = 2.4–24 \text{ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)}\);

\( t_{1/2} = 3.5 \text{ d for reactions with photochemically produced OH radical (Howard 1990)}\);

\( \text{calculated lifetime } \tau = 2.5 \text{ d for reaction with OH radical (Atkinson 2000)}\).

Surface water: volatilization \( t_{1/2} = 11–17 \text{ h from a model river (Howard 1990)}\).

Ground water:

Sediment:

Soil:

Biota:

---

### TABLE 12.1.2.3.1

Reported aqueous solubilities of 2-pentanone at various temperatures

<table>
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<th>Gross et al. 1939</th>
<th>Ginnings et al. 1940</th>
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<td><strong>t/°C</strong></td>
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FIGURE 12.1.2.3.1 Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for 2-pentanone.

TABLE 12.1.2.3.2
Reported vapor pressures of 2-pentanone (methyl propyl ketone) at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947
Collerson et al. 1965
Ambrose et al. 1975(a)

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<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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(Continued)
### TABLE 12.1.2.3.2 (Continued)

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<td>t/°C</td>
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<td>Antoine eq.</td>
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<td>Kirchhoff eq</td>
<td>∆H_v/(kJ mol⁻¹) =</td>
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<td>∆H_v/(kJ mol⁻¹) = 33.64</td>
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</table>

#### FIGURE 12.1.2.3.2

Logarithm of vapor pressure versus reciprocal temperature for 2-pentanone.

2-Pentanone: vapor pressure vs. 1/T

- Collerson et al. 1965
- Ambrose et al. 1974a
- Stull 1947

b.p. = 102.26 °C
12.1.2.4 3-Pentanone

Common Name: 3-Pentanone
Synonym: diethyl ketone, ethylketone, propione, sym-dimethylacetone
Chemical Name: 3-pentanone, diethyl ketone
CAS Registry No: 96-22-0
Molecular Formula: C₆H₁₀O, CH₃CH₂COCH₂CH₃
Molecular Weight: 86.132

Melting Point (°C):
-39  (Lide 2003)

Boiling Point (°C):
101.7  (Gross et al. 1933; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
0.8138  (Weast 1982–83)
0.8143, 0.8095  (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
92.6  (calculated-density, Jaworska & Schultz 1993)
118.4  (calculated-Le Bas method at normal boiling point)

Dissociation Constant:
27.1  (pKₐ, Riddick et al. 1986; Howard 1993)

Enthalpy of Fusion ΔHₘₜₜ (kJ/mol):
11.593  (Riddick et al. 1986)

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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
46900  (30°C, shake flask-interferometer, Gross et al. 1933)
49617*  (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)
49620  (30°C, shake flask-interferometer, Gross et al. 1933)
48100*  (shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)
48100  (shake flask-volumetric, Ginnings et al. 1940)
44520  (shake flask-centrifuge, Booth & Everson 1948)
43170  (estimated, McGowan 1954)
47330  (Deno & Berkheimer 1960)
45650  (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
47000, 38000  (20°C, 100°C, Verschueren 1983)
34000  (20°C, Riddick et al. 1986)
48440*  (calculated-fragment solubility const., Wakita et al. 1986)
53000*  (19.3°C, shake flask-GC, measured range 0–80°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2169*  (interpolated-regression of tabulated data, temp range –12.0 to 103.3°C, Stull 1947)
2666  (27.9°C, Stull 1947)
log (P/mmHg) = 7.25223 – 1450.0/(230 + t°C), (Antoine eq., Dreisbach & Martin 1949)
10114*  (36.36°C, ebulliometry, measured range 36.36–101.7°C, Dreisbach & Shrader 1949)
20441*  (56.649°C, ebulliometry, measured range 56.5–111.3°C, Collerson et al. 1965)
log (P/mmHg) = 7.02742 – 1309.555/(214.118 + t°C); temp range 56.5–111.3°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = 22.02258 – 2614.85/(T/K) – 4.72805·log (T/K); temp range 56.5–111.3°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)
log (P/mmHg) = \[-0.2185 \times 11183.0/(T/K)\] + 9.406280; temp range –12.7–102.7°C, (Antoine eq., Weast 1972–73)

5316, 4714 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.1467 – 1307.941/(213.968 + t°C), temp range 56.53–111.3°C (Antoine eq. from reported expnl. data of Ambrose et al. 1975, Boublik et al. 1984)

log (P/kPa) = 6.13703 – 1349.358/(224.351 + t°C), temp range 36.36–101.7°C (Antoine eq. from reported expnl. data, Boublik et al. 1984)

4932 (Daubert & Danner 1989)

log (P/mmHg) = 32.265 – 2.9431 \times 10^{3}/(T/K) – 8.5068\times \log (T/K) – 4.572 \times 10^{-10}\times (T/K)^2; temp range 234–561 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol):

3.617 (calculated-γP, Rathbun & Tai 1982)

5.340 (calculated-MW, Rathbun & Tai 1982)

8.834 (calculated-P/C, Howard 1993)

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

0.99 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

0.75 (calculated-activity coeff. \(\gamma\), Wasik et al. 1981)

0.67 (calculated-activity coeff. \(\gamma\), Berti et al. 1986)

1.15 (calculated-activity coeff. \(\gamma\) from UNIFAC, Banerjee & Howard 1988)

0.82 (recommended, Sangster 1989, 1993)

0.99 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.519 (estimated-K_{OW}, Lyman et al. 1990; quoted, Howard 1993)

0.146 (estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

1.914 (soil, estimated-K_{OW}, Lyman et al. 1990; quoted, Howard 1993)

1.08 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

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

Volatilization: estimated half-life from a model pond of two meter deep is 5.6 d (USEPA 1987; quoted, Howard 1993); based on calculated Henry’s law constant, estimated \(t_{1/2}\) ~12 h from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

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 \(t_{1/2} = 2.4–24\) h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
Aldehydes and Ketones

\[ k_{\text{OH}} = (1.82 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \pm 2 \text{ K in air (relative rate technique to cyclohexane)} \]

Atkinson et al. 1982

\[ k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

\[ k_{\text{OH}}(\text{obs.}) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)} \]

k_{\text{OH}}(expmt) = 2.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K; experimentally determined } k(\text{soln}) = 2.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)} \]

k_{\text{OH}} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)}

k_{\text{OH}}(\text{calc}) = 3.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1996)}

Hydrolysis: not expected to be important (Howard 1993).

Biodegradation: \( t_{\frac{1}{2}} \approx 5 \text{ to } 10 \text{ d in acclimated cultures during screening tests (Howard 1993).} \)

Biotransformation:

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

Half-Lives in the Environment:

Air: \( t_{\frac{1}{2}} = 2.4\text{–}24\text{ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of}} \)

hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation \( t_{\frac{1}{2}} = 5.9\text{ d, based on an experimentally determined rate constant for the vapor-phase reaction with OH radical in air (Wallington & Kurylo 1987; quoted, Howard 1993).} \)

Surface water: estimated volatilization \( t_{\frac{1}{2}} \approx 12\text{ h in a model river (1 m deep flowing at 1 m/s with a 3 m/s wind)}} \)

and \( t_{\frac{1}{2}} = 5.6\text{ d in a model environmental pond (2 m deep) (Howard 1993).} \)

Ground water:

Sediment:

Soil:

Biota:

---

**TABLE 12.1.2.4.1**

Reported aqueous solubilities of 3-pentanone at various temperatures

<table>
<thead>
<tr>
<th>Gross et al. 1939</th>
<th>Ginnings et al. 1940</th>
<th>Stephenson 1992</th>
</tr>
</thead>
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<tr>
<td>shake flask-IR</td>
<td>volumetric method</td>
<td>shake flask-GC/TC</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>10</td>
<td>67275</td>
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<td>30</td>
<td>49617</td>
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<td>50</td>
<td>39280</td>
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<td></td>
<td>bp/°C</td>
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<td>80.2</td>
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</table>
**FIGURE 12.1.2.4.1** Logarithm of mole fraction solubility (ln $x$) versus reciprocal temperature for 3-pentanone.

**TABLE 12.1.2.4.2**

Reported vapor pressures of 3-pentanone at various temperatures and the coefficients for the vapor pressure equations

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<th>$t$/$^\circ$C</th>
<th>P/Pa</th>
<th>$t$/$^\circ$C</th>
<th>P/Pa</th>
<th>$t$/$^\circ$C</th>
<th>P/Pa</th>
<th>$t$/$^\circ$C</th>
<th>P/Pa</th>
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<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
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<tr>
<td></td>
<td></td>
<td>Stull 1947</td>
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<td>Collerson et al. 1965</td>
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<td>Kirchhoff eq. 4</td>
<td>P/mmHg</td>
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<td>at 25°C</td>
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<td>at bp</td>
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</table>

ΔHV/(kJ mol⁻¹) = 33.72

**FIGURE 12.1.2.4.2** Logarithm of vapor pressure versus reciprocal temperature for 3-pentanone.

3-Pentanone: vapor pressure vs. 1/T
12.1.2.5 Methyl isobutyl ketone (MIBK)

Common Name: Methyl isobutyl ketone
Synonym: hexone, hexanone, 4-methyl-2-pentanone, MIBK
Chemical Name: methyl isobutyl ketone, 4-methyl-2-pentanone
CAS Registry No: 108-10-1
Molecular Formula: C₆H₁₂O, (CH₃)₂CHCH₂COCH₃
Molecular Weight: 100.158

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<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>−84 (Lide 2003)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>116.5 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>0.7978 (Weast 1982–83)</td>
</tr>
<tr>
<td></td>
<td>0.8010 (Riddick et al. 1986)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>125.0 (20°C, calculated-density)</td>
</tr>
<tr>
<td></td>
<td>140.6 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Fusion ΔH_{fus} (kJ/mol)</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion ΔS_{fus} (J/mol K)</td>
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</tr>
<tr>
<td>Fugacity Ratio at 25°C</td>
<td>(assuming ΔS_{fus} = 56 J/mol K), F: 1.0</td>
</tr>
</tbody>
</table>

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):

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Solubility (g/m³ or mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°C</td>
<td>16630*</td>
</tr>
<tr>
<td>20°C</td>
<td>19100*</td>
</tr>
<tr>
<td>20°C</td>
<td>19100</td>
</tr>
<tr>
<td>19.4°C</td>
<td>19200*</td>
</tr>
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</table>

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

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Log (P/mmHg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.7°C</td>
<td>800; 1333</td>
</tr>
<tr>
<td>21.7°C</td>
<td>2200</td>
</tr>
<tr>
<td>22–116°C</td>
<td>2575</td>
</tr>
</tbody>
</table>

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\[
\log (P_{L}/kPa) = 5.79768 - 1168.443/(–81.202 + T/K), \text{ temp range 294–390 K, (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P_{L}/kPa) = 5.83311 - 1188.115/(–79.265 + T/K), \text{ temp range 281–400 K, (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[2687^* \text{ (comparative ebulliometry, extrapolated-Antoine eq., measured range 309.7–416 K, Ambrose et al. 1988)}\]

\[
\ln (p/kPa) = 14.07841 – 3103.029/(T/K – 61.104); \text{ temp range 309.7–416 K (comparative ebulliometry, Ambrose et al. 1988)}
\]

\[
\log (P/mmHg) = 64.1919 – 4.3577 \times 10^3/(T/K) – 19.766 \cdot \log (T/K) – 3.9997 \times 10^{-10} \cdot (T/K)^2; \text{ temp range 189–571 K (vapor pressure eq., Yaws 1994)}
\]

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

\[39.5^* \text{ (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)}\]

\[
\ln [H/(atm m^3/mol)] = –7.157 + 160.6/(T/K), \text{ temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)}
\]

\[9.523 \text{ (calculated-P/C, Howard 1990)}\]

\[47.95^* \text{ (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)}\]

\[
\ln \left(1/K_{AW}\right) = –9.56 + 4237/(T/K), \text{ temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)}
\]

\[45.57 \text{ (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)}\]

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

\[
1.38 \text{ (shake flask-GC, Iwasa et al. 1965)}
\]

\[
1.09 \text{ (calculated-π constant, Hansch et al. 1968)}
\]

\[
1.19 \text{ (Hansch & Leo, 1979)}
\]

\[
1.39 \text{ (HPLC-RT correlation, Haky & Young 1984)}
\]

\[
1.31 \text{ (shake flask-GC, Tanii et al. 1986)}
\]

\[
1.38 \text{ (recommended, Sangster 1993)}
\]

\[
1.31 \text{ (recommended, Hansch et al. 1995)}
\]

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

Bioconcentration Factor, log \(BCF\):

\[
0.301–0.699 \text{ (estimated-} K_{OW} \text{ and S, Lyman et al. 1982; quoted, Howard 1990)}
\]

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

\[
1.279–2.025 \text{ (soil, estimated-} K_{OW} \text{ and S, Lyman et al. 1982; quoted, Howard 1990)}
\]

\[
0.87 \text{ (calculated-} K_{OW}, \text{ Kollig 1993)}
\]

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

Volatilization: \(t_{1/2} = 15–33 \text{ h from water of 1 m deep, based on lab. mass-transfer coefficient for volatilization from a stirred 557–2020 rpm water bath at 25°C (Rathbun & Tai 1982; quoted, Howard 1990).}\)

Photolysis: direct photolysis \(t_{1/2} = 15 \text{ h in air (Howard 1990)}\).

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:

\[
\text{photooxidation } t_{1/2} = 0.24–2.4 \text{ h for the gas-phase reaction with OH radical in air, based on the disappearance rate of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)}
\]

\[
k_{OH} = (0.9 \pm 0.3) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1} \text{ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)}
\]

\[
k_{OH}(calc) = 9.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(obs.) = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)}
\]

\[
\text{photooxidation } t_{1/2} = 4.6–45.5 \text{ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991)}
\]

\[
k_{OH} = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989)}
\]
k_{OH} = (1.31 – 1.45) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} (\text{OH radical concn. of } 8.0 \times 10^5 \text{ molecule cm}^{-3}) \text{ at } 22–27^\circ \text{C},
\text{estimated } t_{1/2} = 16–17 \text{ h (Howard 1990)}

k_{OH(\text{calc})} = 3.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} (\text{molecular orbital calculations, Klamt 1996})

Hydrolysis: not expected to undergo chemical hydrolysis (Howard 1990).

Biodegradation: aqueous aerobic \( t_{1/2} = 24–168 \text{ h} \), based on unacclimated aerobic aqueous screening test data
(Bridie et al. 1979; Takemoto et al. 1981; selected, Howard et al. 1991);
aqueous anaerobic \( t_{1/2} = 96–672 \text{ h} \), 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: \( t_{1/2} = 0.24–2.4 \text{ h} \) for the gas-phase reaction with hydroxyl radical in air, based on the disappearance rate of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
photodecomposition \( t_{1/2} = 3.5 \text{ h} \) under simulated atmospheric conditions, with NO (Dilling et al. 1976);
direct photolysis \( t_{1/2} = 15 \text{ h} \) and photooxidation \( t_{1/2} = 16–17 \text{ h} \) for reactions with hydroxyl radical in air
(Howard 1990);
photooxidation \( t_{1/2} = 4.6–45.5 \text{ h} \), based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: estimated volatilization \( t_{1/2} = 15–33 \text{ h} \) (Howard 1990);
\( t_{1/2} = 24–168 \text{ h} \), based on unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

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

Sediment:

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

Biota:

**TABLE 12.1.2.5.1**

Reported aqueous solubilities of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures

<table>
<thead>
<tr>
<th>Gross et al. 1939</th>
<th>Ginnings et al. 1940</th>
<th>Stephenson 1992</th>
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<tr>
<td><strong>shake flask-IR</strong></td>
<td><strong>volumetric method</strong></td>
<td><strong>shake flask-GC/TC</strong></td>
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<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>0</td>
<td>30749</td>
<td>10</td>
</tr>
<tr>
<td>10</td>
<td>23137</td>
<td>24</td>
</tr>
<tr>
<td>30</td>
<td>16630</td>
<td>30</td>
</tr>
<tr>
<td>50</td>
<td>14123</td>
<td>(bp°C)</td>
</tr>
<tr>
<td>75</td>
<td>13721</td>
<td>115.6–115.7</td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td></td>
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FIGURE 12.1.2.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.2
Reported vapor pressures of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>log P = A − B/(T/K)</th>
<th>ln P = A − B/(T/K)</th>
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<tr>
<td>log P = A − B/(C + t/°C)</td>
<td>ln P = A − B/(C + t/°C)</td>
</tr>
<tr>
<td>log P = A − B/(C + T/K)</td>
<td>ln P = A − B/(C + T/K)</td>
</tr>
<tr>
<td>log P = A − B/(T/K) − C·log (T/K)</td>
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</tr>
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Stull 1947

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<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>
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<tr>
<td>−1.40</td>
<td>133.3</td>
<td>21.7</td>
<td>2200</td>
<td>309.676</td>
<td>4922</td>
</tr>
<tr>
<td>19.7</td>
<td>666.6</td>
<td>32.7</td>
<td>3933</td>
<td>314.495</td>
<td>6239</td>
</tr>
<tr>
<td>30.0</td>
<td>1333</td>
<td>41.4</td>
<td>6266</td>
<td>318.766</td>
<td>7638</td>
</tr>
<tr>
<td>40.8</td>
<td>2666</td>
<td>50.2</td>
<td>9266</td>
<td>324.624</td>
<td>9984</td>
</tr>
<tr>
<td>52.8</td>
<td>5333</td>
<td>60.0</td>
<td>14999</td>
<td>328.196</td>
<td>11607</td>
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<tr>
<td>60.4</td>
<td>7999</td>
<td>70.0</td>
<td>21598</td>
<td>334.215</td>
<td>15105</td>
</tr>
<tr>
<td>70.4</td>
<td>13332</td>
<td>80.1</td>
<td>31997</td>
<td>339.189</td>
<td>18512</td>
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<tr>
<td>85.6</td>
<td>26664</td>
<td>90.9</td>
<td>46396</td>
<td>343.458</td>
<td>21914</td>
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<tr>
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<td>352.107</td>
<td>30381</td>
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<tr>
<td>119.0</td>
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<td>389.35 K</td>
<td>359.039</td>
<td>38940</td>
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<tr>
<td>mp/°C</td>
<td>−84.7</td>
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</table>

Fuge et al. 1952

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<tr>
<th>eq. 4</th>
<th>P/mmHg</th>
<th>A</th>
<th>31.1616</th>
<th>373.360</th>
<th>62819</th>
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<tbody>
<tr>
<td>B</td>
<td>3173.11</td>
<td>379.656</td>
<td>76425</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>−7.7701</td>
<td>383.817</td>
<td>86848</td>
<td></td>
<td></td>
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</tbody>
</table>

Ambrose et al. 1988

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>359.039</td>
<td>38940</td>
</tr>
<tr>
<td>365.854</td>
<td>49155</td>
</tr>
<tr>
<td>369.784</td>
<td>55938</td>
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<tr>
<td>373.360</td>
<td>62819</td>
</tr>
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<td>76425</td>
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<tr>
<td>389.35 K</td>
<td>38940</td>
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<td>400.202</td>
<td>137928</td>
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(Continued)
### TABLE 12.1.2.5.2 (Continued)

<table>
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<tr>
<th>Stull 1947 summary of literature data</th>
<th>Fuge et al. 1952 isoteniscope method</th>
<th>Ambrose et al. 1988 comparative ebulliometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>T/K</td>
</tr>
<tr>
<td>408.620</td>
<td>172120</td>
<td></td>
</tr>
<tr>
<td>415.823</td>
<td>206364</td>
<td></td>
</tr>
<tr>
<td>298.15</td>
<td>2687</td>
<td>(extrapolated)</td>
</tr>
<tr>
<td>eq. 3a</td>
<td>P/kPa</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>14.07841</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>3103.029</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>–61.104</td>
<td></td>
</tr>
</tbody>
</table>

**FIGURE 12.1.2.5.2** Logarithm of vapor pressure versus reciprocal temperature for 4-methyl-2-pentanone.
TABLE 12.1.2.5.3
Reported Henry’s law constants of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and temperature dependence equations

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

Ashworth et al. 1988

<table>
<thead>
<tr>
<th>EPICS-GC</th>
<th>equilibrium headspace-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
</tr>
<tr>
<td>10</td>
<td>66.87</td>
</tr>
<tr>
<td>15</td>
<td>37.49</td>
</tr>
<tr>
<td>20</td>
<td>29.38</td>
</tr>
<tr>
<td>25</td>
<td>39.52</td>
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<tr>
<td>30</td>
<td>68.90</td>
</tr>
<tr>
<td>A</td>
<td>−9.56</td>
</tr>
<tr>
<td>B</td>
<td>160.6</td>
</tr>
</tbody>
</table>

4-Methyl-2-pentanone (MIBK): Henry’s law constant vs. 1/T

FIGURE 12.1.2.5.3 Logarithm of Henry’s law constant versus reciprocal temperature for 4-methyl-2-pentanone.
12.1.2.6 2-Hexanone (Methyl butyl ketone)

Common Name: Methyl butyl ketone
Synonym: 2-hexanone, methyl \( n \)-butyl ketone
Chemical Name: 2-hexanone, methylbutyl ketone
CAS Registry No: 591-78-6
Molecular Formula: \( \text{C}_6\text{H}_{12}\text{O} \), \( \text{CH}_3\text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \)
Molecular Weight: 100.158
Melting Point (°C):
\[-55 \quad \text{(Lide 2003)}\]
Boiling Point (°C):
\[127.6 \quad \text{(Lide 2003)}\]
Density (g/cm\(^3\) at 20°C):
\[0.8113 \quad \text{(Weast 1982–83)}\]
\[0.8113, 0.8067 \quad \text{(20°C, 25°C, Riddick et al. 1986)}\]
Molar Volume (cm\(^3\)/mol):
\[124.2 \quad \text{(calculated-density, Hoy 1970; Amidon & Williams 1982)}\]
\[140.6 \quad \text{(calculated-Le Bas method at normal boiling point)}\]
Dissociation Constant:
\[-8.30 \quad \text{(pK}_a\text{, Riddick et al. 1986)}\]
\[25.30 \quad \text{(pK}_s\text{, Riddick et al. 1986)}\]
Enthalpy of Fusion \( \Delta H_{\text{fus}} \) (kJ/mol):
\[3.56 \quad \text{(Riddick et al. 1986)}\]
Entropy of Fusion \( \Delta S_{\text{fus}} \) (J/mol K):
\[\text{Fugacity Ratio at 25°C (assuming } \Delta S_{\text{fus}} = 56 \text{ J/mol K), F: 1.0}\]

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):
\[14523* \quad \text{(30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)}\]
\[16400* \quad \text{(shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)}\]
\[16400 \quad \text{(shake flask-volumetric, Ginnings et al. 1940)}\]
\[16000 \quad \text{(Erichsen 1952)}\]
\[23930 \quad \text{(shake flask-interferometer, Donahue & Bartell 1952)}\]
\[15870 \quad \text{(estimated, McGowan 1954)}\]
\[16620 \quad \text{(Deno & Berkheimer 1960)}\]
\[35000 \quad \text{(20°C, Verschueren 1983)}\]
\[17500 \quad \text{(20°C, Riddick et al. 1986)}\]
\[15100*, 13700 \quad \text{(19.8°C, 29.7°C, shake flask-GC, measured range 0–91.5°C, Stephenson 1992)}\]

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
\[514.4* \quad \text{(interpolated-regression of tabulated data, temp range 7.7–212.6°C, Stull 1947)}\]
\[\log (P/\text{mmHg}) = [-0.2185 \times 12358.3/(T/\text{K})] + 9.642791; \text{temp range 7.7–127.5°C, (Antoine eq., Weast 1972–73)}\]
\[1549* \quad \text{(ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)}\]
\[509.8 \quad \text{(calculated-Cox eq., Chao et al. 1983)}\]
\[266.6 \quad \text{(20°C, Verschueren 1983)}\]
\[1540 \quad \text{(extrapolated-Antoine eq., Boublik et al. 1984)}\]
\[\log (P/\text{kPa}) = 6.15217 – 1395.406/(208.946 + t/°C), \text{temp range 34.61–154.6°C (Antoine eq. from reported exp. \text{data of Ambrose et al. 1975, Boublik et al. 1984})}\]
\[1549 \quad \text{(Riddick et al. 1986)}\]
\[\log (P/\text{kPa}) = 6.16230 – 1401.738/(209.646 + t/°C), \text{temp range not specified (Antoine eq., Riddick et al. 1986)}\]
\[1715, 1540 \quad \text{(interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)}\]
log (P L/kPa) = 6.4127 − 1575.5/(−43.15 + T/K), temp range 293–411 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.14816 − 1392.968/(−64.465 + T/K), temp range 279–423 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.15949 − 1399.959/(−63.704 + T/K), temp range 310–427 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

1600 (computed-expert system SPARC, Kolling 1995)

log (P/mmHg) = 4.0508 – 2.6276 × 10⁻³/(T/K) + 3.7783·log (T/K) – 1.4342 × 10⁻²·(T/K) + 8.0592 × 10⁻⁶·(T/K)²; temp range 217–587 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol):
9.69 (calculated-P/C, Meylan & Howard 1991)
11.8 (calculated-bond contribution, Meylan & Howard 1991)
9.70 (calculated-P/C, Howard 1993)
8.82 (computed-expert system SPARC, Kolling 1995)

Octanol/Water Partition Coefficient, log Kₐw:
1.38 (shake flask-UV, Iwasa et al. 1965; Leo et al. 1971; Hansch & Leo 1979)
1.29 (calculated-π constant, Hansch et al. 1968)
1.39 (HPLC-k' correlation, Haky & Young 1984)
1.19 (shake flask-GC, Tani et al. 1986)
1.38 (recommended, Sangster 1989, 1993)
1.38 (recommended, Hansch et al. 1995)
1.30 (computed-expert system SPARC, Kolling 1995)

Octanol/Air Partition Coefficient, log Kₐa:
3.68 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.778 (estimated-Kₐw, Lyman et al. 1990)

Sorption Partition Coefficient, log Kₑc:
1.322 (soil, estimated-Kₐw, Lyman et al. 1990)
2.127 (soil, estimated-S, Lyman et al. 1990)
1.10 (computed-Kₐw, Kolling 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: t½ ~ 135 h from a model environmental pond of 2 m deep (USEPA 1987; quoted, Howard 1993); using Henry’s law constant, t½ ~ 12.1 H from a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kₐH for reaction with OH radical, kₐO₃ with NO₃ radical and kₐO₃ with O₃ or as indicated, *data at other temperatures see reference: photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
kₐH = (6.81 ± 0.29) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at (299 ± 2) K (relative rate technique to cyclohexane, Atkinson et al. 1982; quoted, Atkinson 1985)
kₐH(calc) = 7.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, kₐH(obs.) = 8.97 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1985)
kₐH(calc) = 9.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)
kₐH(calc) = 9.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 25°C, which corresponds to a half-life of 42 h at an atmospheric OH- concn of 5 × 10⁶ molecule cm⁻³ (quoted, Howard 1993)
kₐH(calc) = 10.57 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

Hydrolysis:
Biodegradation: half-life of approximately 5 d in acclimated mixed microbial culture (Howard 1993).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2} = 2.4$–$24$ h 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); estimated $t_{1/2} \approx 42$ h for the vapor-phase reaction with OH radical is 42 h at an atmospheric OH- concentration of $5 \times 10^5$ molecule·cm$^{-3}$ (Atkinson 1985; quoted, Howard 1993).
Surface water: volatilization $t_{1/2} = 12.1$ h from a model river, 135 h from a model environmental pond (Howard 1993).
Ground water:
Sediment:
Soil:
Biota:

<table>
<thead>
<tr>
<th>TABLE 12.1.2.6.1</th>
</tr>
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<tbody>
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<td>Reported aqueous solubilities of 2-hexanone at various temperatures</td>
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<td>Gross et al. 1939</td>
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<td>60.5</td>
</tr>
<tr>
<td>70.3</td>
</tr>
<tr>
<td>80.7</td>
</tr>
<tr>
<td>91.5</td>
</tr>
</tbody>
</table>

FIGURE 12.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-hexanone.
TABLE 12.1.2.6.2
Reported vapor pressures of 2-hexanone at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(P/Pa)</th>
<th>Stull 1947</th>
<th>(t/°C)</th>
<th>(P/Pa)</th>
<th>Ambrose et al. 1975(a)</th>
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<tr>
<td>7.7</td>
<td>133.3</td>
<td>34.612</td>
<td>128.935</td>
<td>105328</td>
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<td>28.8</td>
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<td>38.8</td>
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<td>138.034</td>
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<td>26664</td>
<td>59.402</td>
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<td>111.0</td>
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<td>10853</td>
<td>127.583</td>
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<td>127.5</td>
<td>101325</td>
<td>67.976</td>
<td>12972</td>
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</tr>
<tr>
<td>mp/°C</td>
<td>–56.9</td>
<td>72.537</td>
<td>15657</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Antoine eq. for full range:
\[
\begin{align*}
A &= 6.16230 \\
B &= 1401.738 \\
C &= 127.583 \\
\Delta H_f/(kJ mol^{-1}) &= 42.9
\end{align*}
\]

Antoine eq. for restricted range of atmospheric pressure:
\[
\begin{align*}
A &= 6.14801 \\
B &= 1392.870 \\
C &= 127.653 \\
\Delta H_f/(kJ mol^{-1}) &= 36.0
\end{align*}
\]
FIGURE 12.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2-hexanone.
12.1.2.7 2-Heptanone

Common Name: 2-Heptanone
Synonym: methyl n-amyl ketone, methyl pentyl ketone
Chemical Name: 2-heptanone
CAS Registry No: 110-43-0
Molecular Formula: C₇H₁₄O, CH₃(CH₂)₄COCH₃
Molecular Weight: 114.185
Melting Point (°C): –35 (Lide 2003)
Boiling Point (°C): 151.05 (Lide 2003)
Density (g/cm³):
0.81537, 0.81123 (20°C, 25°C, Riddick et al. 1986)
Dissociation Constant:

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. Additional data at other temperatures designated * are compiled at the end of this section):
4300* (25°C, volumetric method, measured range 20–30°C, Ginnings et al. 1940)
4054* (30°C, shake flask-interferometer, measured range 10–75°C, Saylor et al. 1942)
4546 (estimated, McGowan 1954)
4300 (Riddick et al. 1986)
4360* (19.7°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson 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):
521 (interpolated-vapor pressure eq., temp range 4–75°C, Stuckey & Saylor 1940)
\[
\log (P/\text{mmHg}) = 7.36537 – 1650.47/(T/K – 54.48); \text{ temp range 4–75°C (Antoine eq., Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)}
\]
709* (30°C, measured range 10–75°C, Saylor et al. 1942)
133.3* (19.3°C, summary of literature data, temp range 19.3–150.2°C, Stull 1947)
\[
\log (P/\text{mmHg}) = 5.95166 – 1408.13/(194.84 + t/°C); \text{ temp range 36 to 151°C (data fitted to Antoine eq., static method-Ramsay-Young apparatus measurements, Meyer & Wagner 1966)}
\]
\[
\log (P/\text{mmHg}) = [–0.2185 \times 12478.9/(T/K)] + 9.305642, \text{ temp range 19.3–150.2°C, (Antoine eq., Weast 1972–73)}
\]
427* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
\[
\log (P/\text{mmHg}) = [1 – 400.348/(T/K)] \times 10^8\{0.934881 – 4.87941 \times 10^{-1}(T/K) + 4.16258 \times 10^{-7}(T/K)^2\}; \text{ temp range 280.85–400.65 K, (Cox eq., Chao et al. 1983)}
\]
514 (Abraham 1984; Riddick et al. 1986)
504 (extrapolated-Antoine eq., Boublik et al. 1984)
\[
\log (P/kPa) = 6.14611 – 1460.276/(201.636 + t/°C), \text{ temp range 94.7–179.3°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)}
\]
469 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\[
\log (P_k/kPa) = 6.07656 – 1408.73/(–78.31 + T/K), \text{ temp range 303–424 K, (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
log \((P_l/kPa) = 6.15178 - 1464.092/(–71.076 + T/K)\), temp range 327–457 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

\[\log (P_l/kPa) = 6.56718 - 1810.283/(–26.944 + T/K), \text{ temp range } 449–580 K, (\text{Antoine eq.-III, Stephenson & Malanowski 1987})\]

\[\log (P/mmHg) = –13.0256 – 2.6425 \times 10^3/(T/K) + 11.879\cdot\log (T/K) – 2.7571 \times 10^{-2}\cdot (T/K)^2; \text{ temp range } 238–612 K (\text{vapor pressure eq., Yaws 1994})\]

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

14.63 (partial vapor pressure-GC, Buttery et al. 1969)
14.6; 14.94, 14.6 (exptl.; calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
5.715 (calculated-activity coefficient \(\gamma_P\), Rathbun & Tai 1982)
9.120 (calculated-P/C, Mackay & Yuen 1983)
16.0 (correlated-molecular structure, Russell et al. 1992)
17.1 (gas stripping-GC, Shiu & Mackay 1997)

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

2.08 (calculated-activity coefficients, Wasik et al. 1981)
1.98 (generator column-HPLC, Tewari et al. 1982)
2.00 (shake flask-GC, Tani et al. 1986)
2.03 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
1.98 (recommended, Sangster 1993)
1.98 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

Oxidation: 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:

\[k_{OH} = (8.67 \pm 8.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 K (\text{Wallington et al. 1987; quoted, Atkinson 1989})\]

\[k_{OH} = (1.17 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 2 K \text{ with calculated tropospheric lifetime } \tau = 1.0 \text{ d} \text{ (relative rate method, Atkinson et al. 2000)}\]

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetime \(\tau = 1.0 \text{ d}\), based on gas-phase reaction with OH radical (relative rate method, Atkinson et al. 2000)

Surface water:

Ground water:

Sediment:

Soil:

Biota:
### TABLE 12.1.2.7.1
Reported aqueous solubilities of 2-heptanone at various temperatures

<table>
<thead>
<tr>
<th>Ginnings et al. 1940</th>
<th>Saylor et al. 1942</th>
<th>Stephenson 1992</th>
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</thead>
<tbody>
<tr>
<td><strong>volumetric method</strong></td>
<td><strong>shake flask-interferometer</strong></td>
<td><strong>shake flask-GC/TC</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g·m}^{-3} )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>20</td>
<td>4400</td>
<td>10</td>
</tr>
<tr>
<td>25</td>
<td>4300</td>
<td>30</td>
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<tr>
<td>30</td>
<td>4000</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
</tr>
<tr>
<td>( \text{bp/°C} )</td>
<td>151.2–151.3</td>
<td>65</td>
</tr>
<tr>
<td>( d^{25} )</td>
<td>0.8115</td>
<td>75</td>
</tr>
</tbody>
</table>

![2-Heptanone: solubility vs. 1/T](image)

**FIGURE 12.1.2.7.1** Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for 2-heptanone.
TABLE 12.1.2.7.2
Reported vapor pressures of 2-heptanone at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Stuckey &amp; Saylor 1940</th>
<th>Stull 1947</th>
<th>Ambrose et al. 1975(a)</th>
</tr>
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<tbody>
<tr>
<td><strong>static method-Hg manometer</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>comparative ebulliometry</strong></td>
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<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td>data presented as</td>
<td></td>
<td>cont'd</td>
</tr>
<tr>
<td>eq. 3</td>
<td>P/mmHg</td>
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<td>A</td>
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<tr>
<td>B</td>
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</tr>
<tr>
<td>C</td>
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<tr>
<td>Saylor et al. 1942</td>
<td></td>
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<tr>
<td>Stuckey &amp; Saylor data</td>
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<tr>
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<td>30</td>
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<tr>
<td>60</td>
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<tr>
<td>65</td>
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<tr>
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<td>7413</td>
<td></td>
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</tbody>
</table>
| | | | | 112.377 | 31321 | \( \Delta H_v/(kJ \cdot mol^{-1}) = \)
| | | | | 117.486 | 37167 |
| | | | | 117.629 | 37361 |
| | | | | 123.186 | 4713 |
| | | | | 129.297 | 54129 |
| | | | | 134.589 | 63526 |
| | | | | 140.221 | 74904 |
| | | | | 146.323 | 88989 | Antoine eq. for restricted |
| | | | | 150.976 | 101114 |
| | | | | 150.976 | 101114 |
| | | | | 150.976 | 101114 |

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FIGURE 12.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for 2-heptanone.
12.1.2.8 Cyclohexanone

Common Name: Cyclohexanone
Synonym:  
Chemical Name: cyclohexanone
CAS Registry No: 108-94-1
Molecular Formula: \( \text{C}_6\text{H}_{10}\text{O} \)
Molecular Weight: 98.142
Melting Point (\(^{\circ}\)C):
\(-27.9\) (Lide 2003)
Boiling Point (\(^{\circ}\)C):
155.43 (Lide 2003)
Density (g/cm\(^3\) at 20\(^{\circ}\)C):
0.9478 (Weast 1982–83; Dean 1985)
0.9452 (Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
106.2 (calculated-density, Stephenson & Malanowski 1987)
118.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25\(^{\circ}\)C (assuming \(\Delta S_{fus} = 56\) J/mol K), F: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25\(^{\circ}\)C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
23000 (Riddick et al. 1986)
93200 (selected, Yaws et al. 1990)
97000*, 82000 (19.5\(^{\circ}\)C, 29.8\(^{\circ}\)C, shake flask-GC, measured range 0–90.7\(^{\circ}\)C, Stephenson 1992)

Vapor Pressure (Pa at 25\(^{\circ}\)C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
666.6* (26.4\(^{\circ}\)C, summary of literature data, temp range 1.4–155.6\(^{\circ}\)C, Stull 1947)
\[ \log (P/\text{mmHg}) = [–0.2185 \times 10037.6/(T/K)] + 8.019908; \text{ temp range 1.4–155.6}^{\circ}\text{C, (Antoine eq., Weast 1972–73)} \]
533* (ebulliometry-fitted to Antoine eq., temp range 89.6–165.8\(^{\circ}\)C, Meyer & Hotz 1973)
\[ \log (P/\text{mmHg}) = 5.978401 – 1495.511/(209.5117 + t/\text{C}^\circ); \text{ temp range 89.6–165.8}^{\circ}\text{C (Antoine eq. ebulliometric measurements, Meyer & Hotz 1973)} \]
614 (interpolated-Cox eq., Chao et al. 1983)
\[ \log (P/\text{mmHg}) = \{1 – 428.587/(T/K)} \times 10^4\{0.8333332 – 6.42578 \times 10^{-4}.(T/K) + 7.09855 \times 10^{-7}.(T/K)^2\}; \text{ temp range: 274.55–438.92 K (Cox eq., Chao et al. 1983)} \]
533 (extrapolated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{kPa}) = 6.10133 – 1494.166(209.399 + t/\text{C}^\circ), \text{ temp range 89.29–165.8}^{\circ}\text{C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]
640 (Riddick et al. 1986)
\[ \log (P/\text{kPa}) = 6.103304 – 1495.511/(209.5517 + t/\text{C}^\circ), \text{ temp range not specified (Antoine eq., Riddick et al. 1986)} \]
620, 534 (calculated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
\[ \log (P/\text{kPa}) = 8.434 – 2576.6/(T/K); \text{ temp range not specified (Antoine eq., solid, Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 70.5022 – 4.412 \times 10^7/(T/K) – 23.605 \times 10^{-2}.(T/K) – 1.5648 \times 10^{-13}.(T/K)^2; \text{ temp range 242–629 K (vapor pressure eq., Yaws 1994)} \]
Henry’s Law Constant (Pa m$^3$/mol at 25°C):
1.216  (Hawthorne et al. 1985)
2.266  (calculated-P/C, Meylan & Howard 1991)
5.179  (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log $K_{OW}$:
0.81  (shake flask, Hansch & Leo 1979, 1985, 1987)
0.81  (recommended, Sangster 1989, 1993)
0.81  (recommended, Hansch et al. 1995)

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

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

Sorption Partition Coefficient, log $K_{OC}$:
1.00  (calculated-S, $K_{OW}$ with regression eq., Roy & Griffin 1985; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: using Henry’s law constant, $t_{1/2} \approx 3.1$ d from a model river 1-m deep flowing 1 m s$^{-1}$ with wind velocity of 3 m s$^{-1}$ (Lyman et al. 1982; quoted, Howard 1990).
Photolysis: direct sunlight photolysis rate constant of about 0.16 d$^{-1}$ corresponding to $t_{1/2} = 4.3$ d (Mill & Davenport 1986; quoted, Howard 1990).
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 $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
$k_{OH} = 1.56 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C with $t_{1/2} \approx 1$ d (Atkinson 1985; quoted, Howard 1990)
$k_{OH} = 6.39 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1989)
$k_{OH} = 12.55 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ from Atmospheric Oxidation Program, $k_{OH}$(exptl) = $6.39 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{OH}$(calc) = $2.92 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)
$k_{OH}$(calc) = $5.09 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:
Biodegradation: average rate of biodegradation 51.5 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
Half-Lives in the Environment:
Air: $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);
degrade rapidly by reaction with sunlight produced hydroxyl radicals with $t_{1/2} \sim 1$ d and by direct sunlight photolysis with $t_{1/2} \sim 4.3$ d (Howard 1990).
Surface water: estimated $t_{1/2} \sim 0.003$ yr at Noordwijk (Zoeteman et al. 1981).
Ground water:
Sediment:
Soil:
Biota:
TABLE 12.1.2.8.1
Reported vapor aqueous solubilities and vapor pressures of cyclohexanone at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(C + t/°C) \quad (1a) \\
\log P &= A - B/(C + 1/K) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4) \\
\log (P/atm) &= A'\left[1 - \left(T_B/T\right)\right] \quad (5) \\
\text{where } A' &= (a + bT + cT^2)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
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<td></td>
<td>S/g·m⁻³</td>
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</tr>
<tr>
<td>0</td>
<td>137000</td>
<td>1.40 133.3</td>
</tr>
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<td>9.8</td>
<td>115000</td>
<td>26.4 666.6</td>
</tr>
<tr>
<td>19.5</td>
<td>97000</td>
<td>38.7 1333</td>
</tr>
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<td>29.8</td>
<td>82000</td>
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<td>65000</td>
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<td>68000</td>
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<tr>
<td>90.7</td>
<td>69000</td>
<td>155.6 101325</td>
</tr>
<tr>
<td>mp°C</td>
<td>−45.0</td>
<td></td>
</tr>
</tbody>
</table>

Stephenson 1992
-shake flask-GC/TC

Stull 1947
-summary of literature data

Meyer & Hotz 1973
-comparative ebulliometry

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>145.880</td>
<td>78656</td>
</tr>
</tbody>
</table>

Antoine eq.

\[
\text{eq. 2 } \\
A &= 5.978401 \\
B &= 1495.511 \\
C &= 209.5517
\]

Cox eq.

\[
\text{eq. 5 } \\
a &= 0.852046 \\
n-b \times 10^3 &= 0.612660 \\
c \times 10^6 &= 0.504661 \\
T_B/K &= 428.5716
\]
**FIGURE 12.1.2.8.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohexanone.

**FIGURE 12.1.2.8.2** Logarithm of vapor pressure versus reciprocal temperature for cyclohexanone.
12.1.2.9 Acetophenone

Common Name: Acetophenone
Synonym: 1-phenylethanone, methyl phenyl ketone, acetylbenzene, phenylmethylketone, hypnone
Chemical Name: acetophenone, methyl phenyl ketone
CAS Registry No: 98-86-2
Molecular Formula: C₈H₈O, C₆H₅COCH₃
Molecular Weight: 120.149

Melting Point (°C):
20.5 (Stull 1947; Weast 1982–83; Lide 2003)

Boiling Point (°C):
202 (Lide 2003)

Density (g/cm³ at 20°C):
1.0281 (Dreisbach 1955; Weast 1982–83; Riddick et al. 1986)
1.02382 (25°C, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm³/mol):
117.1 (calculated-density, Rohrschneider 1973)
140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):
42.0, 53.41 (normal bp, 25°C, Dreisbach 1955)

Enthalpy of Fusion ∆Hfus (kJ/mol):
16.65 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion ∆Sfus (J/mol K):
42.26 (Tsonopoulos & Prausnitz 1971)

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):
5530 (shake flask-centrifuge, Booth & Everson 1948)
6300 (shake flask-UV, Andrews & Keefer 1950)
6022 (estimated, McGowan 1954)
5540 (24°C, shake flask-LSC, Means et al. 1980)
5500 (Verschueren 1983; Dean 1985, 1992)
6130 (Southworth & Keller 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):
266.6* (50.2°C, static method-manometer, measured range 50.2–201.5°C, Kahlbaum 1898)
66.21* (extrapolated-regression of tabulated data, temp range 37.1–202.4°C, Stull, 1947)
49.53 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.15738 – 1723.46/(201.0 + t°C); temp range 102–330°C (Antoine eq. for liquid state, Dreisbach 1955)
41.30 (Hoy 1970)
log (P/mmHg) = [–0.2185 × 11731.5/(T/K)] + 8.293248; temp range 37.1–202.4°C (Antoine eq., Weast 1972–73)
57.48 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1 – 474.823/(T/K)] × 10^6[0.859974 – 6.15392 × 10⁻⁴(T/K) + 6.99110 × 10⁻⁷(T/K)^²]; temp range 310.25–475.55 K (Cox eq., Chao et al. 1983)
52.92 (Daubert & Danner 1985)
40.23 (extrapolated-Antoine eq., Dean 1985)
Aldehydes and Ketones

\[
\log (P/\text{mmHg}) = 9.1352 - 2878.8/(T/\text{K}); \text{ temp range } 20-100^\circ\text{C} \quad (\text{Antoine eq., Dean 1985, 1992})
\]

\[
49.0 \quad (\text{Riddick et al. 1986})
\]

\[
\log (P/\text{kPa}) = 6.28228 - 1723.46/(201.0 + t/\circ\text{C}), \text{ temp range not specify} \quad (\text{Antoine eq., Riddick et al. 1986})
\]

\[
45.3 \quad (\text{extrapolated-Antoine eq., Stephenson & Malanowski 1987})
\]

\[
\log (P/\text{kPa}) = 6.28228 - 1723.46/(-72.15 + T/\text{K}); \text{ temp range } 375-603 \text{ K} \quad (\text{Antoine eq., Stephenson & Malanowski 1987})
\]

\[
45.00 \quad (\text{selected, Mackay et al. 1992, 1995; quoted, Shiu & Mackay 1997})
\]

\[
\log (P/\text{mmHg}) = 55.5798 - 4.5101 \times 10^3/(T/\text{K}) - 17.284 \times \log (T/\text{K}) + 6.4184 \times 10^{-3} \times (T/\text{K}) + 6.5557 \times 10^{-13} \times (T/\text{K})^2;
\text{ temp range } 293-701 \text{ K} \quad (\text{vapor pressure eq., Yaws 1994})
\]

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

\[
1.082 \quad (\text{calculated-}1/K_{AW}, C_W/C_A, \text{ reported as exptl., Hine & Mookerjee 1975})
\]

\[
0.784 \quad (\text{calculated-bond contribution, Hine & Mookerjee 1975})
\]

\[
0.921^* \quad (25.1^\circ\text{C}, \text{ gas stripping-GC, measured range } 14.9-35^\circ\text{C}, \text{ Betterton 1991})
\]

\[
0.753 \quad (20^\circ\text{C}, \text{ selected from literature experimentally measured data, Staudinger & Roberts 1996})
\]

\[
0.890, 0.982 \quad (\text{gas stripping-GC, calculated-P/C, Shiu & Mackay 1997})
\]

\[
1.06^* \quad (\text{EPICS-UV spectroscopy, measured range } 5-25^\circ\text{C}, \text{ Allen et al. 1998})
\]

\[
\ln K_{AW} = -9100/(T/\text{K}) + 22.47 \quad (\text{EPICS-UV, temp range } 5-25^\circ\text{C}, \text{ Allen et al. 1998})
\]

\[
0.560 \quad (20^\circ\text{C}, \text{ selected from literature experimentally measured data, Staudinger & Roberts 2001})
\]

\[
\log K_{AW} = 7.307 - 3202/(T/\text{K}), \quad (\text{van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001})
\]

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

\[
1.58 \quad (\text{shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1969, 1971; Hansch & Leo 1985})
\]

\[
1.58 \quad (\text{calculated-}\pi \text{ const., Iwasa et al. 1965})
\]

\[
1.73 \quad (\text{shake flask-UV, Chapman et al. 1972})
\]

\[
1.58 \quad (\text{HPLC-RT correlation, Lazare et al. 1974})
\]

\[
1.68 \quad (\text{shake flask-UV, Holmes & Lough 1976})
\]

\[
1.66 \pm 0.08 \quad (\text{shake flask at pH 7, Unger et al. 1978})
\]

\[
1.66 \quad (\text{Hansch & Leo 1979})
\]

\[
1.59 \quad (\text{shake flask-GC, Khan et al 1979})
\]

\[
1.59 \quad (\text{shake flask-LSC, Means et al. 1980})
\]

\[
1.58 \quad (\text{shake flask-HPLC, Nahum & Horvath 1980})
\]

\[
1.75 \quad (\text{calculated-f const., Rekker’s method, Hanai et al. 1981})
\]

\[
1.77, 1.56 \quad (\text{HPLC-}k’ \text{ correlation, McDuffie 1981})
\]

\[
1.80 \quad (\text{HPLC-RT correlation, Hammers et al. 1982})
\]

\[
1.83 \quad (\text{RP-LC-RT correlation, Hanai & Hubert 1982})
\]

\[
1.56 \quad (\text{RP-HPLC-}k’ \text{ correlation, Miyake & Terada 1982})
\]

\[
1.63 \quad (\text{inter-laboratory studies, shake flask average, Eadsworth & Moser 1983})
\]

\[
1.65 \quad (\text{inter-laboratory studies, HPLC average, Eadsworth & Moser 1983})
\]

\[
1.65; 1.68 \pm 0.02 \quad (\text{selected best lit. value; exptl.-ALPM, Garst & Wilson 1984})
\]

\[
1.59; 1.72 \quad (\text{HPLC-RT correlation; HPLC average, Eadsworth 1986})
\]

\[
1.71 \quad (\text{HPLC-RT correlation, Ge et al. 1987})
\]

\[
1.65 \quad (\text{calculated-activity coeff. } \gamma \text{ from UNIFAC, Banerjee & Howard 1988})
\]

\[
1.60 \quad (\text{shake flask-CPC, Berthod et al. 1988})
\]

\[
1.58 \quad (\text{RP-HPLC-}k’ \text{ correlation, Minick et al. 1988})
\]

\[
1.63 \quad (\text{recommended, Sangster 1989, 1993})
\]

\[
1.59 \quad (\text{CPC centrifugal partition chromatography, Gluck & Martin 1990})
\]

\[
1.56 \quad (\text{shake flask-UV spec., Alcorn et al. 1993})
\]

\[
1.58 \quad (\text{recommended, Hansch et al. 1995})
\]

Bioconcentration Factor, log BCF:

\[
0.699-0.954 \quad (\text{estimated-}K_{OW} \text{ and S, Lyman et al. 1982; quoted, Howard 1993})
\]
Sorption Partition Coefficient, log $K_{OC}$:

- 1.544 (average of 3 sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
- 1.380 (calculated, Means et al. 1980)
- 1.89 (calculated-MCI $\chi$, Gerstl & Helling 1987)
- 1.630 (soil, quoted, Sabljic 1987)
- 1.73 (RP-HPLC-k' correlation, cyanopropyl column, Hodson & Williams 1988)
- 1.34–2.43 (soils and sediments, quoted expl. and estimated values, Howard 1993)
- 1.26 (calculated-$K_{OC}$, Kollig 1993)
- 1.54 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
- 1.79, 1.63 (RP-HPLC-k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.61, 1.50, 1.80 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 1.56, 1.55 (sediments: 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: based on calculated Henry’s law constant, $t_{1/2} \approx 3.8$ d from a model river of 1-m deep flowing at 1 m s$^{-1}$ with a wind velocity of 3 m s$^{-1}$ (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, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{OH} = (2.74 \pm 0.15) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1989)
  - $k_{OH}^{(calc)} = 1.61 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ estimated from Atmospheric Oxidation Program; $k_{OH}^{(exptl)} = 2.74 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ estimated from Fate of Atmospheric Pollutants Program with OH radical in vapor phase (Meylan & Howard 1993)
  - $k_{OH}^{(calc)} = 0.74 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(exptl)} = 2.74 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)
- Hydrolysis:
- Biodegradation: biodegradation rate constant $k = 0.029–0.042$ h$^{-1}$ in 30 mg L$^{-1}$ activated sludge after a time lag of 15–20 h (Uranp & Kato 1986b);
  - rate constants: $k = 0.022$ d$^{-1}$ in ground water, $k = 0.083$ d$^{-1}$ in river waters and $k = 0.155$ d$^{-1}$ in Superior harbor waters (Vaishnav & Babeu 1987).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: estimated photooxidation $t_{1/2} \approx 22$ d in atmosphere, based on the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson 1988; quoted, Howard 1993); atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).
- Surface water: biodegradation $t_{1/2} = 8$ d in river water and $t_{1/2} = 4.5$ d in lake water (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993) and $t_{1/2} = 4$ d in Superior harbor waters (Vaishnav & Babeu 1987).
- Ground water: biodegradation $t_{1/2} = 32$ d (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993); estimated $t_{1/2} \approx 0.01$ yr at Noordwijk (Zoeteman et al. 1981).
### TABLE 12.1.2.9.1
Reported aqueous solubilities and Henry's law constants of acetophenone at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stephenson 1992</td>
<td>Betterton 1991</td>
</tr>
<tr>
<td>Allen et al. 1998</td>
<td>EPICS-UV</td>
</tr>
<tr>
<td>shake flask-GC/TC</td>
<td>gas stripping-GC</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
</tr>
<tr>
<td>19.9</td>
<td>5620</td>
</tr>
<tr>
<td>29.5</td>
<td>7100</td>
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<tr>
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<tr>
<td>60.1</td>
<td>8880</td>
</tr>
<tr>
<td>70.2</td>
<td>9920</td>
</tr>
<tr>
<td>80.1</td>
<td>12040</td>
</tr>
</tbody>
</table>

$\Delta H/(kJ\ mol^{-1}) = -50.5$

$\ln K_{AW} = A - B/(T/K)$

**Acetophenone: solubility vs. $1/T$**

**FIGURE 12.1.2.9.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for acetophenone.
## TABLE 12.1.2.9.2
Reported vapor pressures of acetophenone at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Kahlbaum 1898</th>
<th>Stull 1947</th>
</tr>
</thead>
<tbody>
<tr>
<td>static method-manometer*</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>(t/°C)</td>
<td>(P/Pa)</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>50.2</td>
<td>266.6</td>
</tr>
<tr>
<td>56.0</td>
<td>400.0</td>
</tr>
<tr>
<td>61.0</td>
<td>533.3</td>
</tr>
<tr>
<td>65.0</td>
<td>666.6</td>
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<td>79.0</td>
<td>1333.2</td>
</tr>
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<td>87.3</td>
<td>1999.8</td>
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<td>93.4</td>
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<td>102.4</td>
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<td>109.7</td>
<td>5332.9</td>
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<td>114.7</td>
<td>6666.1</td>
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<td>66661</td>
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<td>192.5</td>
<td>79993</td>
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<td>198.5</td>
<td>93326</td>
</tr>
<tr>
<td>201.5</td>
<td>101325</td>
</tr>
</tbody>
</table>

*complete list see ref.

**FIGURE 12.1.2.9.2** Logarithm of Henry’s law constant versus reciprocal temperature for acetophenone.
FIGURE 12.1.2.9.3 Logarithm of vapor pressure versus reciprocal temperature for acetophenone.
12.1.2.10 Benzophenone

![Benzophenone structure](image)

Common Name: Benzophenone
Synonym: diphenyl ketone, diphenyl methanone
Chemical Name: benzophenone, diphenyl ketone
CAS Registry No: 119-61-9
Molecular Formula: C\textsubscript{13}H\textsubscript{10}O, C\textsubscript{6}H\textsubscript{5}COC\textsubscript{6}H\textsubscript{5}
Molecular Weight: 182.217

Melting Point (°C):
- 48.1 (α, Weast 1982–83; Dean 1985)
- 26.0 (β, Weast 1982–83; Dean 1985)
- 47.9 (Lide 2003)

Boiling Point (°C):
- 305.4 (Lide 2003)

Density (g/cm\textsuperscript{3} at 20°C):
- 1.6077 (α, 19°C, Weast 1982–83)
- 1.6059 (β, 23°C, Weast 1982–83)
- 1.111 (18°C, Lide 2003)

Molar Volume (cm\textsuperscript{3}/mol):
- 206.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Vaporization, ΔH\textsubscript{v} (kJ/mol):
- 53.38, 81.90 (normal bp, 25°C, Dreisbach 1955)

Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):
- 16.99 (Dreisbach 1955)
- 13.36 (Yalkowsky & Valvani 1980)

Entropy of Fusion ΔS\textsubscript{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS\textsubscript{fus} = 56 J/mol K), F: 0.596 (mp at 47.9°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 20720, 21000 (calculated-ΔS\textsubscript{fus} and mp, estimated, Yalkowsky & Valvani 1980)
- 276 (calculated-intrinsic molar volume V\textsubscript{i} and solvatochromic parameters, Leahy 1986)
- 77.7 (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):

- 33330* (257.15°C, temp range 257.15–302.85°C, Jaquerod & Wassenh 1904; quoted, Boublik et al. 1984)
- 0.617* (extrapolated-regression tabulated data, temp range 108.3–305.5°C, Stull 1947)

\[ \log (P/\text{mmHg}) = 7.81086 - 2643.0/(230 + t/°C) \] (Antoine eq., Dreisbach & Martin 1949)

\[ 6287* (200.50°C, ebulliometry, measured range 200.50–306.1°C, Dreisbach & Shrader 1949) \]

1.242 (calculated by formula, Dreisbach 1955)

\[ \log (P/\text{mmHg}) = 7.28937 - 2144.6/(181.0 + t/°C); \text{ temp range 1980–600°C} \] (Antoine eq. for liquid state, Dreisbach 1955)

\[ \log (P/\text{mmHg}) = [-0.2185 \times 14725.4/(T/K)] + 8.456678; \text{ temp range 108.2–305.4°C} \] (Antoine eq., Weast 1972–73)

3.146* (55.9°C, effusion method, measured range 55.9–71.2°C, DePablo 1976)

0.086, 0.0115 (extrapolated-Antoine eq., Boublik et al. 1984)

\[ \log (P/\text{kPa}) = 6.2931 – 2056.386/(173.545 + t/°C); \text{ temp range 200.5–306.1°C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1984)

\[ \log (P/\text{kPa}) = 6.37814 – 2127.915/(181.209 + t/°C); \text{ temp range 257.1–302.8°C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1984)
Aldehydes and Ketones

0.080 (extrapolated-Antoine eq., Dean 1985)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 7.34966 - \frac{2331.4}{(195.0 + t/\degree C)}, \text{ temp range } 48-202\degree C \] (Antoine eq., Dean 1985, 1992)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 7.16294 - \frac{2051.855}{(173.074 + t/\degree C)}; \text{ temp range } 200-306\degree C \] (Antoine eq., Dean 1985, 1992)

0.086, 0.095 (interpolated-eq.-I and II, Stephenson & Malanowski 1987)

\[ \log \left( \frac{P}{\text{kPa}} \right) = 16.4144 - 3.8064 \times 10^3/(T/\text{K}) - 2.3984 \times 10^{-3} \log (T/\text{K}) - 7.4544 \times 10^{-7} \times (T/\text{K})^2; \text{ temp range } 321-816 K \] (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol):

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

- 3.18 (shake flask-UV, Leo et al. 1971)
- 3.58 (shake flask-UV, Holmes & Lough 1976)
- 3.10 (shake flask-UV, Unger & Chiang 1981)
- 3.02 (HPLC-‘k’ correlation, McDuffie 1981)
- 3.03 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 3.18 (recommended, Sangster 1989, 1993)
- 3.18 (recommended, Hansch et al. 1995)
- 3.09 (microemulsion electrophoresis-retention factor correlation, Poole et al. 2000)

Bioconcentration Factor, \( \log BCF \):

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

- 2.63 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Half-Lives in the Environment:
### TABLE 12.1.2.10.1
Reported vapor pressures of benzophenone at various temperatures and the coefficients for the vapor pressure equations

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

Jaquerod & Wassher 1904
Stull 1947
Dreisbach & Shrader 1949
DePablo 1976

<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>257.15</td>
<td>33330</td>
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<td>133.3</td>
<td>200.50</td>
<td>6287</td>
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<td>666.6</td>
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<td>7605</td>
<td>60.7</td>
<td>4.280</td>
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Jaquerod, A. Wassher, E. Ber. 3, 2531 (1904)

**FIGURE 12.1.2.10.1** Logarithm of vapor pressure versus reciprocal temperature for benzophenone.
# 12.2 SUMMARY TABLES AND QSPR PLOTS

## TABLE 12.2.1
Summary of physical properties of aldehydes and ketones

<table>
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<tr>
<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p. °C</th>
<th>b.p. °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Molar volume, $V_m$ cm³/mol</th>
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<td>152.8</td>
<td>1</td>
<td>140.41**</td>
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* Assuming $\Delta S_{\text{ fus }} = 56 \text{ J/mol K}$; # at 18°C; ** at 25°C.
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<th>Selected properties</th>
<th>Vapor pressure</th>
<th>log K&lt;sub&gt;OW&lt;/sub&gt; calc P/C</th>
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<th>exptl (b)</th>
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(a) Butler et al. 1935, Buxton et al. 1969; (b) Zhou & Mopper 1990; (c) Snider & Dawson 1985; (d) Betterton & Hoffmann 1988.
### TABLE 12.2.3
Suggested half-life classes for aldehydes and ketones at various environmental compartments at 25°C

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<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
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<td>3</td>
<td>4</td>
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<td>4</td>
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<td>2-Butenal</td>
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where,

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<th>Range (hours)</th>
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<td>10–30</td>
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<td>3</td>
<td>55 (~ 2 days)</td>
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</tr>
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<td>4</td>
<td>170 (~ 1 week)</td>
<td>100–300</td>
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<td>5</td>
<td>550 (~ 3 weeks)</td>
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<tr>
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<td>5,500 (~ 8 months)</td>
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<td>8</td>
<td>17,000 (~ 2 years)</td>
<td>10,000–30,000</td>
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<tr>
<td>9</td>
<td>~ 5 years</td>
<td>&gt; 30,000</td>
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</table>
FIGURE 12.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.

FIGURE 12.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.
FIGURE 12.2.3 Octanol-water partition coefficient versus Le Bas molar volume for aldehydes and ketones.

FIGURE 12.2.4 Henry's law constant versus Le Bas molar volume for aldehydes and ketones.
FIGURE 12.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aldehydes and ketones.
12.3 REFERENCES


Aldehydes and Ketones

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Aldehydes and Ketones


13 Carboxylic Acids

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13.1 LIST OF CHEMICALS AND DATA COMPILATIONS

13.1.1 ALIPHATIC ACIDS

13.1.1.1 Formic acid

![Formic acid structure]

Common Name: Formic acid
Synonym: methanoic acid
Chemical Name: formic acid
CAS Registry No: 64-18-6
Molecular Formula: CH$_2$O$_2$, HCOOH
Molecular Weight: 46.026
Melting Point (°C):
- 8.3 (Lide 2003)
Boiling Point (°C):
- 101 (Lide 2003)
Density (g/cm$^3$ at 20°C):
- 1.2161, 1.21328 (20°C, 25°C, Dreisbach & Martin 1949)
- 1.2200 (Weast 1982–83; Dean 1985)
- 1.2141 (25°C, Riddick et al. 1986)
Molar Volume (cm$^3$/mol):
- 37.7 (calculated-density, Stephenson & Malanowski 1987)
- 46.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK$_a$:
- 3.751 (pK$_a$, Dean 1985)
- 3.752 (pK$_a$, Riddick et al. 1986)
- 3.740 (pK$_a$, Sangster 1989)
- 3.800 (Kollig 1993)
Enthalpy of Fusion, ∆H$_{fus}$ (kJ/mol):
- 12.68 (Riddick et al. 1986)
Entropy of Fusion, ∆S$_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S$_{fus}$ = 13.5 J/mol K), F: 1.0
Water Solubility (g/m$^3$ or mg/L at 25°C):
- miscible (Dean 1985)
- miscible (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):
- 4344* (24.6°C, temp range 21.8–100.6°C, Kahlbaum 1894)
- 5333* (24°C, compiled and evaluated data, temp range –20 to 100.6°C, Stull 1947)
\[
\log (P/\text{mmHg}) = 7.15689 - 1414.1/(230 + t/°C) \quad (\text{Antoine eq., Dreisbach & Martin 1949})
\]
- 10114* (37.75°C, ebulliometry, measured range 37.75–100.7°C, Dreisbach & Shrdar 1949)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 9896.5/(T/K)] + 8.779337; \text{temp range –20 to 100.6°C (Antoine eq., Weast 1972–73)}
\]
- 4666, 7198 (20°C, 30°C, Verschueren 1983)
- 5720, 5744, 4420 (calculated-Antoine eq., Boublik et al. 1984)
\[
\log (P/\text{kPa}) = 4.09278 - 539.775/(136.826 + t/°C) \quad (\text{Antoine eq. from reported exptl. data, Boublik et al. 1984})
\]
\[
\log (P/\text{kPa}) = 6.69157 - 1689.096/(259.726 + t/°C) \quad (\text{Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984})
\]
\[
\log (P/\text{kPa}) = 3.7279 - 295.021/(70.7 + t/°C) \quad (\text{Antoine eq. from reported exptl. data, Boublik et al. 1984})
\]
Log (P/mmHg) = 7.5818 – 1699.2/(260.7 + t°C); temp range: 37–101°C (Antoine eq., Dean 1985, 1992)

Log (P/kPa) = 6.5028 – 1563.28/(–26.09 + T/K); temp range 283–384 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Log (P/mmHg) = 7.5818 – 1699.2/(260.7 + t°C); temp range not specified (Antoine eq., Dean 1986)

Log (P/kPa) = 11.611 – 3160/(T/K); temp range 268–281 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

Log (P/kPa) = 6.5028 – 1563.28/(247.06 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

Log (P/mmHg) = 27.9278 – 2.5976 × 10³/(T/K) – 7.2489·log (T/K) + 6.411 × 10⁻¹⁰·(T/K) + 3.9421 × 10⁻⁶·(T/K)²; temp range 282–580 K (vapor pressure eq., Yaws 1994)

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

0.0181 (calculated, Keene & Galloway 1986)
0.0274 (calculated, Jacob 1986)
0.017 (pH 4, Gaffney et al. 1987)
0.112 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
0.0076, 0.0098, 0.0178 (24°C, bubble column technique, concn: of 1, 10, 10⁵ ppm, Servant et al. 1991)
0.0281 (Bettermont 1992)
0.018 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

Log [kH/(mol kg⁻¹ atm⁻¹)] = –10.31 + 5634/(T/K), temp range 178.15–308.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0183 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
0.018–0.028 (calculated-thermodynamic data, Johnson et al. 1996)
0.0118, 0.00921 (counter-flow packed column technique-ion chromatography; “best” exptl. value, Johnson et al. 1996)

Log [kH(M/atm)] = –11.04 + 6100/(T/K); temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)

0.0137 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
0.0107 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
Log K₆₆ = 2.914 – 2425/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K₆₆:

–0.54 (shake flask-titration, Collander 1951; quoted, Leo et al. 1971; Hansch et al. 1972; Hansch & Leo 1979)
–0.54 (shake flask-titration, Whitehead & Geankoplis 1955)
–0.46 (calculated-f const., Rekker & de Kort 1979)
–0.54 (recommended, Sangster 1989)
–0.54 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K₆₆:

–0.27 (calculated-K₆₆, Kollig 1993)

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

Volatileization:

Photolysis:

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

$k_{\text{OH}} = (3.2 \pm 1.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982)

$k = (100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ at pH 8; $(5 \pm 5) \text{ M}^{-1} \text{ s}^{-1}$ for protonated species; $(100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0–4.0 and 20–23°C (Hoigné & Bader 1983b)

$k_{\text{OH}*} = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–430 K (flash photolysis-resonance fluorescence, Wine et al. 1985)

$k_{\text{OH}} = (2.95 \pm 0.07) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance absorption, Jolly et al. 1986)

$k_{\text{OH}} = (3.7 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{\text{OH}*} = (2.69 \pm 0.17) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297–445 K, measured range 297–445 K (laser photolysis-resonance absorption, Singleton et al. 1988)

$k_{\text{OH}} = 3.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}} = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}*} = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 13.1.1.1.1</th>
<th>Reported vapor pressures of formic acid at various temperatures and the coefficients for the vapor pressure equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\log P = A − B/(T/K)$ (1)</td>
<td>$\ln P = A − B/(T/K)$ (1a)</td>
</tr>
<tr>
<td>$\log (P/mmHg) = A − B/(C + t/°C)$ (2)</td>
<td>$\ln (P/mmHg) = A − B/(C + t/°C)$ (2a)</td>
</tr>
<tr>
<td>$\log (P/Pa) = A − B/(C + T/K)$ (3)</td>
<td>$\ln (P/Pa) = A − B/(C + T/K)$ (3a)</td>
</tr>
<tr>
<td>$\log (P/mmHg) = A − B/(T/K) − C\log (T/K)$ (4)</td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Kahlbaum 1894</th>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shadrer 1949</th>
<th>Ambrose &amp; Ghassee 1987</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ber. 16, 2476</td>
<td>summary of literature data</td>
<td>ebulliometry</td>
<td>comparative ebulliometry</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
<td>$P/Pa$</td>
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<tr>
<td>21.8</td>
<td>3312</td>
<td>-20.0</td>
<td>133</td>
</tr>
<tr>
<td>22.6</td>
<td>3688</td>
<td>-5.0</td>
<td>666.6</td>
</tr>
<tr>
<td>24.6</td>
<td>4344</td>
<td>2.10</td>
<td>1333</td>
</tr>
<tr>
<td>27.9</td>
<td>5520</td>
<td>10.3</td>
<td>2666</td>
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<td>30.5</td>
<td>6621</td>
<td>24.0</td>
<td>5333</td>
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<td>37.8</td>
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<td>100.6</td>
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<td>80.3</td>
<td>53329</td>
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<td></td>
<td></td>
<td>100.6</td>
<td>101325</td>
</tr>
<tr>
<td></td>
<td></td>
<td>mp/°C</td>
<td>8.2</td>
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</tbody>
</table>

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### TABLE 13.1.1.1.1 (Continued)

<table>
<thead>
<tr>
<th></th>
<th>Kahlbaum 1894</th>
<th>Stull 1947</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Ambrose &amp; Ghiassee 1987</th>
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<td></td>
<td><strong>summary of literature data</strong></td>
<td><strong>ebulliometry</strong></td>
<td><strong>comparative ebulliometry</strong></td>
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</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>T/K</strong></td>
</tr>
<tr>
<td>350.313</td>
<td>47321</td>
<td>↓↓</td>
<td>353.362</td>
<td>52449</td>
</tr>
<tr>
<td>353.362</td>
<td>52449</td>
<td>↓↓</td>
<td>355.215</td>
<td>55868</td>
</tr>
<tr>
<td>392.654</td>
<td>172035</td>
<td>↓↓</td>
<td>298.15</td>
<td>5733</td>
</tr>
<tr>
<td><strong>Antoine eq.</strong></td>
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<tr>
<td><strong>eq. 3a</strong></td>
<td><strong>P/kPa</strong></td>
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<tr>
<td><strong>A</strong></td>
<td>15.40560</td>
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<tr>
<td><strong>B</strong></td>
<td>3894.764</td>
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<td></td>
</tr>
<tr>
<td><strong>C</strong></td>
<td>–13.0</td>
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<tr>
<td><strong>bp/K</strong></td>
<td>374.04</td>
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</tr>
</tbody>
</table>

**FIGURE 13.1.1.1.1** Logarithm of vapor pressure versus reciprocal temperature for formic acid.

Formic acid: vapor pressure vs. 1/T

- b.p. = 101 °C
- m.p. = 8.3 °C
13.1.1.2 Acetic acid

Common Name: Acetic acid
Synonym: ethanoic acid, methanecarboxylic acid, glacial acetic, vinegar acid
Chemical Name: acetic acid
CAS Registry No: 64-19-7
Molecular Formula: CH₃COOH
Molecular Weight: 60.052
Melting Point (°C):
16.64 (Lide 2003)
Boiling Point (°C):
117.9 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
1.04923, 1.04365 (20°C, 25°C, Dreisbach & Martin 1949)
1.0492 (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
57.1 (calculated-density, Rohrschneider 1973)
68.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
4.733 (pKₐ, Korman & La Mer 1936)
4.760 (pKₐ, Fieser & Fieser 1958; Sangster 1989)
4.750 (pKₐ, Weast 1982–83; Howard 1990)
4.756 (pKₐ, Dean 1985; Riddick et al. 1986)
Enthalpy of Fusion, ΔH₉ (kJ/mol):
11.72 (Ambrose et al. 1977; 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):
miscible (Dean 1985; Riddick et al. 1986)
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):
2040* (interpolated-regression of tabulated data, temp range –17.2–118°C, Stull 1947)
log (P/mmHg) = 7.45144 – 1589.3/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
10114* (55.75°C, ebulliometry, measured range 55.75–117.72°C, Dreisbach & Shrader 1949)
2666* (29.8°C, static method-manometer, measured range 29.8–126.45°C, Potter & Ritter 1954)
8297* (52.36°C, ebulliometry, measured range 52.36–118.14°C, McDonald et al. 1959)
log (P/mmHg) = 7.55716 – 1642.54/(233.386C + t/°C); temp range 52–118°C (ebulliometry, McDonald et al. 1959)
2105 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.18807 – 1416.7/(211 + t°C), temp range 36–170°C, (Antoine eq. for liquid state, Dreisbach 1961)
2030 (Hoy 1970)
log (P/mmHg) = [–0.2185 × 9963.9/(T/K)] + 8.50200; temp range –35 to 10°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9486.6/(T/K)] + 8.142405; temp range –17.2 to 312.5°C (Antoine eq., Weast 1972–73)
2079* (ebulliometry, fitted to Antoine eq., measured range 304.065–415.041 K, Ambrose et al. 1977)
log (P/kPa) = 6.66686 – 1633.288/((T/K) – 40.626); temp range 351.347–415.041 K (Antoine eq.-I, ebulliometry, Ambrose et al. 1977)
log (P/kPa) = 6.59795 – 1587.182/(T/K – 45.392); temp range 304.065–126.45°C (Antoine eq.-II, ebulliometry, Ambrose et al. 1977)

2050, 32660 (measured, calculated-solvatochromic parameters., Banerjee et al. 1990)

log (P/mmHg) = 7.38782 – 1533.313/(222.309 + t°C), temp range: liquid (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 28.3756 – 2.9734 × 10³/(T/K) – 7.032·log (T/K) – 1.5051 × 10⁻⁹·(T/K)²; temp range 290–593 K (vapor pressure eq., Yaws 1994)

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

0.0303 (partial pressure, Butler & Ramchandani 1935)
0.0305 (exptl., Hine & Mookerjee 1975)
0.0300, 0.0280 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.0115 (calculated, Keene & Galloway 1986)
0.0101 (effective Henry’s law constant, pH 4, Gaffney et al. 1987)
0.0254 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
0.121 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
0.0101, 1.01 × 10⁻² (at pH 4, pH 7, Howard 1990)
0.0109, 0.00905, 0.0158 (23°C, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)
0.0184 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
ln [K_H/(mol kg⁻¹ atm⁻¹)] = −25.67 + 8322/(T/K), temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
0.0285 (calculated-bond contribution, Brimblecombe et al. 1992)
0.0431 (calculated-molecular structure, Russell et al. 1992)
0.0182 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
0.0115–0.0195 (calculated-thermodynamic data, Johnson et al. 1996)
0.0245, 0.0145 (counter-flow packed column technique-ion chromatography; “best” exptl value, Johnson et al. 1996)
\[ \ln \left[ \frac{K_p}{(M/\text{atm})} \right] = -12.5 + \frac{6200}{(T/\text{K})}, \quad \text{temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)} \]

- 0.0130 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)
- 0.0154 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

\[ \log K_{\text{AW}} = 3.650 - \frac{2596}{(T/\text{K})} \] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
- -0.30 (shake flask-titration, Leonard et al. 1948)
- -0.31 (shake flask-titration, Collander 1951)
- -0.29; -0.17 (calculated-fragment const.; calculated-\( \pi \) const., Rekker 1977)
- -0.29 (shake flask-radiochemical method, pH 1, Woffenden 1978)
- -0.17, -0.31 (Hansch & Leo 1979)
- -0.17 (shake flask, Log P Database, Hansch & Leo 1987)
- -0.17 (recommended, Sangster 1989, 1993)
- -0.17 (recommended, Hansch et al. 1995)

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

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

Sorption Partition Coefficient, \( \log K_{\text{OC}} \):
- no detectable sorption (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 0.00 (soil, quoted exptl., Meylan et al. 1992)
- -0.21 (soil, calculated-MCI \( \gamma \) and fragment contribution, Meylan et al. 1992)
- 0.00 (soil, calculated-MCI \( \gamma \), 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, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO3}} \) with NO3 radical and \( k_{\text{O3}} \) with O3 or as indicated, *data at other temperatures see reference:

\( k_{\text{OH}} = (0.6 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with \( t_{1/2} = 26.7 \text{ d} \) for the vapor-phase reaction with \( 5 \times 10^5 \) hydroxyl radical/cm³ in air at 25°C (flash photolysis-resonance fluorescence technique, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

\( k(\text{aq.}) \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1} \) for reaction with ozone at pH 8 in water; \( k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1} \) for protonated species, and \( k \leq 3 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1} \) for non-protonated species for the reaction with ozone in water at pH 2.0–5.5 and 20–23°C (Hoigne & Bader 1983b)

\( k_{\text{OH}}^\# = (7.4 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K, measured range 298–440 K (flash photolysis-resonance fluorescence, Dagaut et al. 1988)

\( k_{\text{OH}} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) in air, and \( k(\text{soln}) = 2.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

\( k_{\text{OH}} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Atkinson 1990)

\( k_{\text{OH}}(\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (molecular orbital calculations, Klamt 1996).

Hydrolysis:

Biodegradation: > 90% degradation in 3 d using an activated sludge inoculum; in 24 h in batch aeration in sewage and 14 d using sediment from the Rhine river as inocula (Howard 1990).

Biotransformation:

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

Half-Lives in the Environment:

Air: \( t_{1/2} = 26.7 \text{ d} \), based on measured rate constant of \( 0.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the vapor-phase reaction with \( 5 \times 10^5 \) hydroxyl radicals/cm³ in air at 25°C (Atkinson 1985; quoted, Howard 1990).

Surface water: \( t_{1/2} = 26–46 \text{ yr} \), based on OH radical concn. in sunlit natural water of \( 1 \times 10^{-17} \text{ mol/L} \) (Howard 1990).
Groundwater:
Sediment: > 90% degradation in 14 d using Rhine River sediment as inocula (Kool 1984; quoted, Howard 1990).
Soil:
Biota:

**TABLE 13.1.1.2.1**
Reported vapor pressures of acetic acid at various temperatures and the coefficients for the vapor pressure equations

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<th>P (Pa)</th>
<th>Temperature (°C)</th>
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<td>Dreisbach &amp; Shrader 1949</td>
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<td>McDonald et al. 1959</td>
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<td>static method-manometer</td>
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Antoine eq.

- eq. 2
- P/mmHg
- A = 7.4275
- B = 1558.03
- C = 224.79

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FIGURE 13.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for acetic acid.
13.1.1.3 Propionic acid

Common Name: Propionic acid
Synonym: methylacetic acid, propanoic acid
Chemical Name: propanoic acid, propionic acid
CAS Registry No: 79-09-4
Molecular Formula: C₃H₆O₂, CH₃CH₂COOH
Molecular Weight: 74.079
Melting Point (°C): –20.5 (Lide 2003)
Boiling Point (°C): 141.15 (Lide 2003)
Density (g/cm³ at 20°C): 0.99336, 0.98797 (20°C, 25°C, Dreisbach & Martin 1949), 0.9930 (Weast 1982–83)
Molar Volume (cm³/mol): 74.6 (20°C, calculated-density), 90.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pkₐ: –6.80 (pK value, Perrin 1972), 4.874 (Dean 1985; Riddick et al. 1986), 4.870 (Sangster 1989)
Enthalpy of Fusion, ΔHfus (kJ/mol): 10.66 (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)

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):
550* (interpolated-regression of tabulated data, temp range 4.6–141.4°C, Stull 1947)
log (P/mmHg) = 7.92234 – 1869.4/(230 + t°C), (Antoine eq., Dreisbach & Martin 1949)
7605* (72.39°C, ebulliometry, measured range 72.39–140.80°C, Dreisbach & Shrader 1949)
446 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.35027 – 1497.4775/(194.12 + t°C), temp range 60–185°C (Antoine eq., Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 12454.4/(T/K)] + 9.647835; temp range 4.6–238°C (Antoine eq., Weast 1972–73)
435* (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
log (P/kPa) = 6.64344 – 1594.723/[T(K) – 70.545]; temp range 328–438 K (Antoine eq., ebulliometry, Ambrose et al. 1981)
500, 442 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.84202 – 1736.007/(218.032 + t°C), temp range 72.39–123.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.67457 – 1615.227/(204.788 + t°C), temp range 55.11–164.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
257 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 6.403 – 950.2/(130.3 + t°C), temp range 56–139.5°C (Antoine eq., Dean 1985, 1992)
451 (Riddick et al. 1986)
log (P/kPa) = 6.64334 – 1594.273/(202.605 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)
452 (comparative ebulliometry, Ambrose & Ghassee 1987)
\[
\ln \left( \frac{P}{kPa} \right) = 15.29686 - \frac{3670.949}{[T/K] - 70.545}, \text{ (Antoine eq., Ambrose \\& Ghiassee 1987)}
\]
\[
\log \left( \frac{P}{L/kPa} \right) = 6.60267 - \frac{1577.96}{79.844 + T/K}, \text{ temp range 343–419 K (Antoine eq.-I, Stephenson \\& Malanowski 1987)}
\]
\[
\log \left( \frac{P}{L/kPa} \right) = 9.24101 - \frac{12835.99}{23.07 + T/K}, \text{ temp range 414–511 K (Antoine eq.-II, Stephenson \\& Malanowski 1987)}
\]
\[
453, 8758 \text{ (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)}
\]
\[
\log \left( \frac{P}{mmHg} \right) = 20.2835 - \frac{3.1165 \times 10^3}{T/K} - 3.6015 \cdot \log (T/K) - 1.3892 \times 10^{-3} \cdot (T/K) + 7.1801 \times 10^{-7} \cdot (T/K)^2; \text{ temp range 252–604 K (vapor pressure eq., Yaws 1994)}
\]
\[
14560^* \text{ (88.37°C, VLE still-manometry, measured range 88.37–140.59°C, Clifford et al. 2004)}
\]
\[
\ln \left( \frac{P}{kPa} \right) = 18.105654 - \frac{5640.3443}{(t/°C) + 277.46143}; \text{ temp range 88.37–140.59°C (Antoine eq., VLE still-
\text{manometry, Clifford et al. 2004)}
\]

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0445 (partial pressure, Butler \\& Ramchandani 1935)
0.0450 (exptl., Hine \\& Mookerjee 1975)
0.0420, 0.0430 (calculated-group contribution, calculated-bond contribution, Hine \\& Mookerjee 1975)
0.0298 (calculated-MCI $\chi$, Nirmalakhandan \\& Speece 1988)
0.0163, 0.00151, 0.0289 (23.1°C, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)
0.0180 (equilibrium partial pressure, Khan \\& Brimblecombe 1992)
0.0431 (calculated-bond contribution, Brimblecombe et al. 1992)
0.0177 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$:
0.25 (shake flask-titration, Collander 1951)
0.23, 0.24 (calculated-$\pi$ const., calculated-fragment const., Rekker 1977)
0.33, 0.25 (Hansch \\& Leo 1979)
0.27 (shake flask-titration, Umland 1983)
0.33 (recommended, Sangster 1989; 1994)
0.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:
Sorption Partition Coefficient, $\log K_{oc}$:

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

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO₃ radical and $k_O_3$ with O₃ as indicated, *data at other temperatures see reference:
$k_{OH} = (1.6 \pm 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (flash photolysis-resonance fluorescence, Zetzsch \\& Stuhl 1982; quoted, Atkinson 1985)
$k = 2.0 \times 10^{-13}$ M⁻¹ s⁻¹ for reaction with ozone at pH 8 in water, $k \leq 4.0 \times 10^{-4}$ M⁻¹ s⁻¹ for protonated species, and $k = (1 \pm 0.5) \times 10^{-3}$ M⁻¹ s⁻¹ for non-protonated species for the reaction with ozone in water at pH 2–5 and 20–23°C (Hoigné \\& Bader 1983b)
$k_{OH}* = (1.22 \pm 0.12) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988)
$k_{OH} = 1.22 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ in air and $k(\text{soln}) = 1.0 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)
$k_{OH} = (1.22 - 1.60) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1989)
$k_{OH}^{(\text{calc})} = 1.35 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

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

Half-Lives in the Environment:
TABLE 13.1.1.3.1
Reported vapor pressures of propionic acid at various temperatures and the coefficients for the vapor pressure equations

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

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

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<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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**Stull 1947**

**Dreisbach & Shrader 1949**

**Ambrose et al. 1981**

**Clifford et al. 2004**

**summary of literature data**

**ebulliometry**

**comparative ebulliometry**

**VLE still-Hg manometer**

**data also fitted to Wagner equations**

**data also fitted to Chebyshev and Wagner equations**

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FIGURE 13.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propionic acid.
13.1.1.4  Butyric acid

Common Name: Butyric acid
Synonym: butanoic acid, n-butyric acid, ethylacetic acid
Chemical Name: n-butyric acid, butyric acid
CAS Registry No: 107-92-6
Molecular Formula: C₄H₈O₂, CH₃CH₂CH₂COOH
Molecular Weight: 88.106
Melting Point (°C):
-5.1  (Lide 2003)
Boiling Point (°C):
163.75  (Lide 2003)
Density (g/cm³ at 20°C):
0.95767, 0.95273  (20°C, 25°C, Dreisbach & Martin 1949)
0.9582  (Dean 1985; Riddick et al. 1986)
Molar Volume (cm³/mol):
92.0  (20°C, calculated-density)
112.8  (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
4.817  (Dean 1985)
4.822  (Riddick et al. 1986)
4.820  (Sangster 1993)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
11.6  (Riddick et al. 1986)
Entropy of Fusion, ∆S_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_fus = 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)
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*  (25.5°C, temp range 25.5–163.5°C, Stull 1947)
log (P/mmHg) = 8.19524 – 2089.9/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
4716*  (90.92°C, ebulliometry, measured range 90.92–163.25°C, Dreisbach & Shrader 1949)
95.77  (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.38423 – 1542.6/(179.9 + t°C), temp range 82–210°C, (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 11881.2/(T/K)] + 8.773450; temp range 25.5–352°C (Antoine eq., Weast 1972–73)
83.95*  (comparative ebulliometry, fitted to Antoine eq., measured range 340–452 K, Ambrose et al. 1981)
104.92  (extrapolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 6.8682 – 1766.906/(200.097 + t°C), temp range 90.2–163.25°C (Antoine eq. from reported exptrl. data, Boublík et al. 1984)
log (P/kPa) = 6.67596 – 1642.683/(188.013 + t°C); temp range 76.53–178.9°C (Antoine eq. from reported exptrl. data, Boublík et al. 1984)
104.3  (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.7399 – 1764.7/(199.9 + t°C); temp range 90–163°C (Antoine eq., Dean 1985, 1992)
102.0  (selected, Riddick et al. 1986)
log (P/kPa) = 6.55643 – 1563.444/(179.843 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)

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ln (P/kPa) = 15.09674 – 3599.963/(T/K – 93.307), (Antoine eq. from previous comparative ebulliometry measurements, Ambrose & Ghiassee 1987)

log (P L/kPa) = 6.50913 – 1542.6/(–94.15 + T/K); temp range 355–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (PL/kPa) = 7.3554 – 2180.05/(–29.337 + T/K); temp range 437–592 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P L/kPa) = 11.53324 – 5291.631/(128.778 + T/K); temp range 301–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 8.0847 – 3.3219 × 10^3/(T/K) + 2.4312·log (T/K) – 1.1734 × 10^-2·(T/K) + 5.7992 × 10^-6·(T/K)^2; temp range 268–628 K (vapor pressure eq., Yaws 1994)

ln (P/kPa) = 14.511627 – 3164.4707/(t/°C) + 156.56122; temp range 110.4–162.9°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

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

0.0542 (partial pressure, Butler & Ramchandani 1935)
0.0542; 0.0590; 0.0650 (expil.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
0.0375 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
0.0222 (equilibrium partial pressure, Khan & Brimblecombe 1992)
0.0654 (calculated-bond contribution, Brimblecombe et al. 1992)
0.358 (calculated-molecular structure, Russell et al. 1992)
0.0211 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, log K$_{ow}$:

0.79 (shake flask-TN, Collander 1951)
0.94 (calculated-TSA, Iwase et al. 1985)
0.824, 0.70 (calculated-CLOGP, calculated-M.O., Bodor et al. 1989)
0.79 (recommended, Sangster 1993)
0.79 (recommended, Hanch 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$_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

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

k$_{OH}$ = (2.4 ± 0.7) × 10^−12 cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K was determined using (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985, 1989)

k(apparent) ≤ 4 × 10^−2 M$^{-1}$ s$^{-1}$ for reaction with ozone at pH 8 in water, k ≤ 6.0 × 10^−3 M$^{-1}$ s$^{-1}$ for protonated species, and k ≤ 6.0 × 10^−3 M$^{-1}$ s$^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–4 and 20–23°C (Hoigné & Bader 1983b)

k$_{OH}$ = 1.80 × 10^−12 cm$^3$ molecule$^{-1}$ s$^{-1}$ in air and k(soln) = 3.70 × 10^−12 cm$^3$ molecule$^{-1}$ s$^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

k$_{OH}$(calc) = 3.11 × 10^−12 cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_{1}$) and Elimination (k$_{2}$) Rate Constants:
### TABLE 13.1.1.4.1

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

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<td>t/°C</td>
<td>P/Pa</td>
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**Antoine eq.**

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<td>C</td>
<td>156.56122</td>
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Data also fitted to Chebyshev and Wagner equations

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FIGURE 13.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for butyric acid.
13.1.1.5 Isobutyric acid

Common Name: Isobutyric acid
Synonym: isobutanoic acid, \textit{i}-butyric acid, 1-butyric acid, dimethylacetic acid, 2-methylpropionic acid, isopropylformic acid
Chemical Name: \textit{i}-butyric acid, isobutyric acid
CAS Registry No: 79-31-2
Molecular Formula: C\textsubscript{4}H\textsubscript{8}O\textsubscript{2}, (CH\textsubscript{3})\textsubscript{2}CHCOOH
Molecular Weight: 88.106
Melting Point (°C):
-46.0 (Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
154.45 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.9490 (Verschueren 1983)
0.9682 (Riddick et al. 1986)
Molar Volume (cm\textsuperscript{3}/mol):
92.7 (20°C, calculated-density, Stephenson & Malanowski 1987)
112.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK\textsubscript{a}:
4.860 (Riddick et al. 1986)
Enthalpy of Fusion, \Delta H\textsubscript{fus} (kJ/mol):
5.02 (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):
228000 (20°C, synthetic method, Jones 1929)
200000 (20°C, quoted, Verschueren 1983)
170000 (Dean 1985)
228000 (20°C, 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):
273.8* (interpolated-regression of tabulated data, temp range 14.7–154.5°C, Stull 1947)
185 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.40246 – 1529.2/(185.0 + t°C), temp range 73–190°C, (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 \times 11182.8/(T/K)] + 8.55228; temp range 14.7–336°C (Antoine eq., Weast 1972–73)
185.0 (Riddick et al. 1986)
184* (comparative ebulliometry, measured range 344.3–445.6 K, Ambrose & Ghiassie 1987)
\ln (P/kPa) = 15.31143 – 3695.332/[(T/K) – 82.0]; temp range 344.3–447 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghiassie 1987)
257.2 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P\textsubscript{T}/kPa) = 7.20794 – 202.52/(-38.649 + T/K); temp range 288–428 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P\textsubscript{T}/kPa) = 7.11635 – 206.61/(-35.297 + T/K), temp range 428–562 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 11.3037 – 3.1625 \times 10^{3}/(T/K) + 0.7263\log (T/K) – 8.9331 \times 10^{-3}(T/K) + 4.8215 \times 10^{-6}(T/K)^{2}; temp range 227–609 K (vapor pressure eq., Yaws 1994)
14550* (102.6°C, VLE still-manometer, measured range 102.6–153.01°C, Clifford et al. 2004)
\[
\ln (P/\text{kPa}) = \frac{15.176238 - 3527.8614}{(t/°C) + 180.5140}; \text{ temp range 102–153.01°C (Antoine eq., VLE still-
manometry, Clifford et al. 2004)}
\]

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

- 0.0178, 0.0289, 0.0633 (23.7°C, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)
- 0.0897 (equilibrium partial pressure, Khan & Brimblecombe 1992)
- 0.0899 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

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

- 0.50, 1.13 (calculated, Verschueren 1983)
- 0.94 (recommended, Sangster 1993)
- 1.10 (at pH 3.5, quoted, Hansch et al. 1995)

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

Bioconcentration Factor, \(\log B\text{CF}\):

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

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

- Volatilization:
- Photolysis:
- Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{oh}}\) for reaction with OH radical, \(k_{\text{no3}}\) with NO₃ radical and \(k_{\text{O}}\) with O, as indicated, *data at other temperatures see reference:
  - \(k_{\text{oh}}^* = (2.0 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988; Atkinson 1989)
  - \(k_{\text{oh}}(\text{calc}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) (molecular orbital calculations, Klamt 1996)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants:

Half-Lives in the Environment:

**TABLE 13.1.1.5.1**

Reported vapor pressures of isobutyric acid (2-methyl propanoic acid) at various temperatures and the coefficients for the vapor pressure equations

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### TABLE 13.1.1.5.1 (Continued)

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**FIGURE 13.1.1.5.1** Logarithm of vapor pressure versus reciprocal temperature for isobutyric acid.
13.1.1.6  *n*-Valeric acid

[Chemical structure image]

Common Name: *n*-Valeric acid  
Synonym: pentanoic acid, valeric acid  
Chemical Name: *n*-valeric acid, valeric acid  
CAS Registry No: 109-52-4  
Molecular Formula: C_5H_{10}O_2, CH_3CH_2CH_2CH_2COOH  
Molecular Weight: 102.132  
Melting Point (°C):  
–33.6  (Lide 2003)  
Boiling Point (°C):  
186.1  (Lide 2003)  
Density (g/cm³ at 20°C):  
0.9391  (Weast 1982–83)  
0.9390  (Dean 1985; Riddick et al. 1986)  
Molar Volume (cm³/mol):  
108.4  (20°C, calculated-density, Stephenson & Malanowski 1987)  
135.0  (calculated-Le Bas method at normal boiling point)  
Dissociation Constant, pKᵢ:  
4.820  (18°C, Weast 1982–83)  
4.860  (Riddick et al. 1986)  
4.830  (Sangster 1989, 1993)  
Enthalpy of Fusion, ΔHₕₜₚ (kJ/mol):  
14.17  (Riddick et al. 1986)  
Entropy of Fusion, ΔSₕₜₚ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₕₜₚ = 56 J/mol K), F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
26000  (20°C, quoted, Amidon et al. 1975)  
24000  (Verschueren 1983; Dean 1985)  
24000  (20°C, 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):  
39.6*  (extrapolated-regression of tabulated data, temp range 42.2–184.4°C, Stull 1947)  
18.75  (calculated by formula, Dreisbach 1961)  
log (P/mmHg) = 7.57366 – 1694.3/(175.0 + t/°C), temp range 102–250°C, (Antoine eq. for liquid state, Dreisbach 1961)  
log (P/mmHg) = [−0.2185 × 13370.3/(T/K)] + 9.271178; temp range 42.2–184.4°C (Antoine eq., Weast 1972–73)  
20.0  (20°C, Verschueren 1983)  
4.33, 6.37 (extrapolated-Antoine eq., Boublik et al. 1984)  
log (P/kPa) = 4.58366 – 609.613/(62.754 + t°C); temp range 72.4–173.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
log (P/kPa) = 5.0835 – 878.669/(95.711 + t°C); temp range 81.1–116.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
log (P/mmHg) = 5.412 – 591/(60 + t°C); temp range 72–174°C (Antoine eq., Dean 1985, 1992)  
19.0  (Riddick et al. 1986)  
log (P/kPa) = 6.7818 – 1777.2/(186.6 + t°C), temp range not specified (Antoine eq., Riddick et al. 1986)  
21.0*  (comparative ebulliometry, measured range 372.5–465.3 K, Ambrose & Ghiassie 1987)  
ln (P/kPa) = 15.25555 – 3811.202/[T/(K) − 101.0], temp range 372.5–456.3 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghiassie 1987)  
16.9  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log \( (P_i/kPa) = 6.69856 – 1694.37/(–98.15 + T/K) \), temp range 375–523 K (Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/mmHg) = 15.3454 –3.9024 \times 10^3/(T/K) – 0.024353 \cdot \log (T/K) – 1.1099 \times 10^{-2} \cdot (T/K)^2; \\
\text{temp range 239–651 K (vapor pressure eq., Yaws 1994)}
\]

14560 \( (130^\circ C, \text{VLE still-manometer, measured range 130–178.77\degree C, Clifford et al. 2004}) \)

\[
\ln (P/kPa) = 36.410366 – 30029.229/[(t/\degree C) + 760.44819]; \text{temp range 130–178.77\degree C (Antoine eq., VLE still-manometry, Clifford et al. 2004)}
\]

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):

0.0478 \( \) (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

\[
\ln [K_{\text{eq}}/(\text{mol kg}^{-1} \cdot \text{atm}^{-1})] = –15.37 + 6879/(T/K); \text{temp range 278.15–308.15 K. (equilibrium partial pressure, Khan & Brimblecombe 1992)}
\]

0.0618, 0.0989 \( \) (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0448* \( \) (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

\[
\ln [K_{\text{eq}}/(\text{mol kg}^{-1} \cdot \text{atm}^{-1})] = –14.3371 + 6582.96/(T/K); \text{temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)}
\]

0.0310 \( \) (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.030 \( \) (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

log \( K_{\text{AW}} = 4.861 – 2865/(T/K) \) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.42 \( \) (Scherrer & Howard 1979)

0.99, 1.69 \( \) (calculated, Verschueren 1983)

1.39 \( \) (recommended, Sangster 1993)

1.39 \( \) (recommended, Hansch et al. 1995)

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, \( t_{1/2} \):

Half-Lives in the Environment:

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<td>\text{VLE still-manometry}</td>
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<td>( P/Pa )</td>
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<td>( P/Pa )</td>
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<tr>
<td>93.1</td>
<td>2666</td>
<td>384.489</td>
<td>6125</td>
</tr>
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</table>

(Continued)
TABLE 13.1.1.6.1 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>116.6</td>
<td>7999</td>
<td>398.670</td>
<td>11637</td>
<td>163.33</td>
<td>49780</td>
<td>ln H = A - B/(T/K)</td>
</tr>
<tr>
<td>128.3</td>
<td>13332</td>
<td>404.759</td>
<td>15006</td>
<td>168.74</td>
<td>59850</td>
<td>A = -14.3371</td>
</tr>
<tr>
<td>146.0</td>
<td>26664</td>
<td>414.079</td>
<td>21807</td>
<td>173.30</td>
<td>69920</td>
<td>B = 6582.96</td>
</tr>
<tr>
<td>165.0</td>
<td>53329</td>
<td>422.753</td>
<td>30285</td>
<td>175.33</td>
<td>74960</td>
<td></td>
</tr>
<tr>
<td>184.4</td>
<td>101325</td>
<td>429.637</td>
<td>55786</td>
<td>17720</td>
<td>79990</td>
<td></td>
</tr>
<tr>
<td>mp/°C</td>
<td>-34.5</td>
<td>449.980</td>
<td>76308</td>
<td>454.060</td>
<td>86528</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>460.052</td>
<td>101592</td>
<td>405.378</td>
<td>120678</td>
<td></td>
</tr>
</tbody>
</table>

Antoine eq.

eq. 2a

A = 36.410366
B = 30029.229
C = 760.44819

data also fitted to Wagner eq.

mp/°C = 34.5

FIGURE 13.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for n-valeric acid.
FIGURE 13.1.1.6.2 Logarithm of Henry's law constant versus reciprocal temperature for n-valeric acid.
13.1.1.7 Hexanoic acid (Caproic acid)

Common Name: Hexanoic acid
Synonym: butylacetic acid, caproic acid, \( n \)-hexanoic acid
Chemical Name: butylacetic acid, hexanoic acid, \( n \)-hexanoic acid
CAS Registry No: 142-62-1
Molecular Formula: \( C_6H_{12}O_2, \ CH_3(CH_2)_3CH_2COOH \)
Molecular Weight: 116.158
Melting Point (°C):
-3 \text{ (Lide 2003)}
Boiling Point (°C):
205.2 \text{ (Lide 2003)}
Density (g/cm\(^3\) at 20°C):
Dissociation Constant, \( pK_a \):
4.850 \text{ (Dean 1985; Bintein & Devillers 1994)}
4.879 \text{ (Riddick et al. 1986)}
4.870 \text{ (Sangster 1989, 1993)}
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
15.4 \text{ (Riddick et al. 1986)}
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \), F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
9887 \text{ (Valvani et al. 1981)}
11000 \text{ (Verschueren 1983)}
10816 \text{ (Windholz 1983)}
6391 \text{ (calculated-activity coefficient } \gamma \text{ from UNIFAC, Banerjee 1985)}
9580 \text{ (20°C, 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):
133.3* \text{ (71.4°C, summery of literature data, temp range 71.4–202°C, Stull 1947)}
\log (P/\text{mmHg}) = [-0.2185 \times 16189.4/(T/K)] + 10.431464; \text{ temp range 71.4–202°C (Antoine eq., Weast 1972–73)}
4.40 \text{ (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)}
\log (P/\text{kPa}) = 6.76323 – 1789.425/(T/K) – 101.930; \text{ temp range: 386.3–441.8 K (Antoine eq., ebulliometry, Ambrose et al. 1981)}
26.7 \text{ (20°C, Verschueren 1983)}
9.92, 1.65 \text{ (extrapolated-Antoine eq., Boublik et al. 1984)}
\log (P/\text{kPa}) = 6.74777 – 1779.677/(127.391 + t/°C), \text{ temp range 98.1–179.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\log (P/\text{kPa}) = 6.06182 – 1347.897/(127.391 + t/°C), \text{ temp range 98.1–179.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\log (P/\text{kPa}) = 6.9249 – 1340.8/(126.6 + t/°C), \text{ temp range 98–179°C (Antoine eq., Dean 1985, 1992)}
5.00 \text{ (Riddick et al. 1986)}
\log (P/\text{kPa}) = 6.76323 – 1789.425/(171.22 + t/°C), \text{ temp range not specified (Antoine eq., Riddick et al. 1986) 6.0 (calculated from Wagner eq. derived from experimental data, Ambrose & Ghiassiee 1987)}
\ln (P/\text{kPa}) = 15.30352 – 3957.396/(T/K) – 108 \text{ (Antoine eq., Ambrose & Ghiassiee 1987)}
\log (P/\text{mmHg}) = 7.08241 – 2009.93/(–82.69 + T/K); \text{ temp range 335–487 K (Antoine eq., Stephenson & Malanowski 1987)}
log (P/mmHg) = 55.7058 − 5.6602 × 10^3/(T/K) − 15.458 log (T/K) + 1.0823 × 10^{-9}(T/K)^2;

temp range 270–667 K (vapor pressure eq., Yaws 1994)

9520 (140.25°C, VLE still-manometer, measured range 140.25–178.28°C, Clifford et al. 2004)

ln (P/kPa) = 13.46595 − 2642.198/[t/°C + 95.20133]; temp range 140.25–178.28°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

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

0.0768 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

ln [K_H/(mol kg^{-1} atm^{-1})] = −12.69 + 5988/(T/K); temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0873, 0.149 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0720* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

ln [K_H/(mol kg^{-1} atm^{-1})] = −13.9424 + 6303.73/(T/K); temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0583 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0556 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 3.955 − 2520/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.88 (Scherrer & Howard 1979)

1.87 (HPLC-RT correlation, D’Amboise & Hanai 1982)

1.92 (shake flask-titration, Umland 1983)

2.09 (shake flask-fluorescence, Nishimura et al. 1985)

1.32 (calculated-activity coefficient γ from UNIFAC, Banerjee & Howard 1988)

2.03 ± 0.01 (potentiometric titration, Hersey et al. 1989)

1.92 (recommended, Sangster 1989, 1993)

1.92 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.38; 1.42; 1.57 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)

1.46; 0.88 (soil, quoted expl.; calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.46 (soil, calculated-MCI 1χ, Sabljic et al. 1995)

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

Half-Lives in the Environment:
### TABLE 13.1.1.7.1
Reported vapor pressures and Henry's law constants of hexanoic acid (caproic acid) at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Vapor pressure</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T/K</td>
<td>P/Pa</td>
</tr>
<tr>
<td></td>
<td>T/K</td>
<td>P/Pa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>71.4</td>
<td>133.3</td>
<td>386.270</td>
</tr>
<tr>
<td>89.5</td>
<td>666.6</td>
<td>388.571</td>
</tr>
<tr>
<td>99.5</td>
<td>1333</td>
<td>391.485</td>
</tr>
<tr>
<td>111.8</td>
<td>2666</td>
<td>395.428</td>
</tr>
<tr>
<td>125.0</td>
<td>5333</td>
<td>398.865</td>
</tr>
<tr>
<td>133.3</td>
<td>7999</td>
<td>402.913</td>
</tr>
<tr>
<td>144.0</td>
<td>13332</td>
<td>406.610</td>
</tr>
<tr>
<td>160.8</td>
<td>26664</td>
<td>410.665</td>
</tr>
<tr>
<td>181.0</td>
<td>53329</td>
<td>414.581</td>
</tr>
</tbody>
</table>

mp/°C | -1.5 | 418.705 | 13001 | Antoine eq. |

|          |        |        |        | eq. 2     |
|          |        |        |        | P/kPa     |
|          |        |        |        | A         |
|          |        |        |        | B         |
|          |        |        |        | C         |
|          |        |        |        | data also fitted to Wagner eq. |

data also fitted to Wagner eq.

![Graph](image-url)

**FIGURE 13.1.1.7.1** Logarithm of vapor pressure versus reciprocal temperature for hexanoic acid.
FIGURE 13.1.1.7.2 Logarithm of Henry's law constant versus reciprocal temperature for hexanoic acid.
13.1.1.8 Stearic acid (Octadecanoic acid)

Common Name: Stearic acid
Synonym: octadecanoic acid
Chemical Name: stearic acid, octadecanoic acid, n-octadecylic acid
CAS Registry No: 57-11-4
Molecular Formula: C₁₈H₃₆O₂, CH₃(CH₂)₁₆COOH
Molecular Weight: 284.478
Melting Point (°C): 69.3 (Lide 2003)
Boiling Point (°C): 350 (dec., Lide 2003)
Density (g/cm³ at 20°C): 0.9408 (Weast 1982–83)
Molar Volume (cm³/mol):
  335.9 (70°C, Stephenson & Malanowski 1987)
  423.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
  4.50 (estimated, Sangster 1989)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
Entropy of Fusion, ∆Sfus (J/mol K):
  39.57; 43.5 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.368 (mp at 69.3°C)
Water Solubility (g/m³ or mg/L at 25°C):
  340 (Verschueren 1983)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  133.3 (173.7°C, summary of literature data, temp range:173.7–370°C, Stull 1947)
  log (P/mmHg) = [–0.2185 × 19306.6/(T/K)] + 9.457471; temp range:173.7–370°C, (Antoine eq., Weast 1972–73)
  1.69 × 10⁻¹² (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.17126 – 2157.5/(–153.78 + T/K); temp range 349–415 K (Antoine eq-I., Stephenson & Malanowski 1987)
  log (P/kPa) = 5.85188 – 1717.93/(–201.829 + T/K); temp range 447–649 K (Antoine eq-II., Stephenson & Malanowski 1987)
  log (P/mmHg) = –40.3638 – 4.7724 × 10³/(T/K) + 24.502·log (T/K) – 3.7665 × 10⁻²·(T/K) + 1.4595 × 10⁻⁵·(T/K)²;
temp range 343–799 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log Kₐw:
  8.23 (HPLC-RT correlation, D’Amboise & Hanai 1982)
  8.23 (recommended, Sangster 1989, 1993)
Octanol/Air Partition Coefficient, log Kₐa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₒₒ:
Environmental Fate Rate Constants, k or Half-Lives, t½:
Half-Lives in the Environment:
13.1.1.9 Oleic acid

Common Name: Oleic acid
Synonym: cis-9-octadecenoic acid, (Z)-9-octadecenoic acid
Chemical Name: oleic acid
CAS Registry No: 112-80-1
Molecular Formula: C₁₈H₃₄O₂, CH₃(CH₂)₇CH=CH(CH₂)₉CH₂COOH
Molecular Weight: 282.462
Melting Point (°C):
13.4 (Lide 2003)
Boiling Point (°C):
360 (Lide 2003)
Density (g/cm³ at 20°C):
0.8870 (25°C, Riddick et al. 1986)
0.8935 (Lide 2003)
Molar Volume (cm³/mol):
314.7 (Stephenson & Malanowski 1987)
416.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
5.02 (Riddick et al. 1986)
4.50 (Sangster 1989)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
Entropy of Fusion, ΔSₘₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
insoluble (McBain & Richards 1946; Riddick et al. 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
133 (178.5°C, summary of literature data, temp range 176.5–360°C, Stull 1947)
0.00144 (extrapolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 20326.7/(T/K)] + 9.930301; temp range 176.5–360°C (Antoine eq., Weast 1972–73)
0.00113 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/Pa) = 8.22018 – 3711.59/(–36.125 + T/K); temp range 444–635 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 78.6973 – 8.8227 × 10³/(T/K) – 22.472-log (T/K) + 4.8353 × 10⁻¹¹(T/K) + 2.6578 × 10⁻⁶(T/K)²;
temp range 287–633 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₐₙw:
7.64 (RP-HPLC-k’ correlation, D’Amboise & Hanai 1982)
7.64 (recommended, Sangster 1989, 1993)
Octanol/Air Partition Coefficient, log Kₐₙa:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log Kₖₐː
13.1.1.10 Acrylic acid (2-Propenoic acid)

\[
\begin{align*}
\text{Common Name: } & \text{Acrylic acid} \\
\text{Synonym: } & \text{acroleic acid, ethylenecarboxylic acid, 2-propenoic acid, propenoic acid} \\
\text{Chemical Name: } & \text{acrylic acid, 2-propenoic acid, propenoic acid} \\
\text{CAS Registry No: } & 79-10-7 \\
\text{Molecular Formula: } & C_3H_4O_2, \text{CH}_2\text{=CHCOOH} \\
\text{Molecular Weight: } & 72.063 \\
\text{Melting Point (°C): } & 12.5 \text{ (Lide 2003)} \\
\text{Boiling Point (°C): } & 141 \text{ (Lide 1003)} \\
\text{Density (g/cm}^3\text{ at 20°C): } & 1.0511 \text{ (Weast 1982–83; Dean 1985; Riddick et al. 1986)} \\
\text{Molar Volume (cm}^3\text{/mol): } & 68.9 \text{ (calculated-density, Stephenson & Malanowski 1987)} \\
& 83.2 \text{ (calculated-Le Bas method at normal boiling point)} \\
\text{Dissociation Constant, } & pK_a \\
& -4.41 \text{ (Perrin 1972)} \\
& 4.25 \text{ (pK}_a, \text{Weast 1982–83)} \\
& 4.26 \text{ (pK}_a, \text{Dean 1985)} \\
& 4.255 \text{ (pK}_a, \text{Riddick et al. 1986)} \\
\text{Enthalpy of Fusion, } & \Delta H_{\text{fus}} \text{ (kJ/mol): } 11.13 \text{ (Riddick et al. 1986)} \\
\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: 1.0 \\
\text{Water Solubility (g/m}^3\text{ or mg/L at 25°C): } & \text{miscible (Dean 1985)} \\
& \text{miscible (Riddick et al. 1986)} \\
& \text{miscible (Yaws et al. 1990)} \\
\text{Vapor Pressure (Pa at 25°C and reported temperature dependence equations): } \\
& 570.8 \text{ (interpolated-regression of tabulated data, temp range 3.5–141°C, Stull 1947)} \\
& 506.5 \text{ (Hoy 1970)} \\
& 570 \text{ (interpolated-Antoine eq., Weast 1972–73)} \\
& \log (P/\text{mmHg}) = [-0.2185 \times 10955.1/(T/K)] + 8.659704; \text{ temp range 3.5–141°C (Antoine eq., Weast 1972–73)} \\
& 426.6 \text{ (20°C, Verschueren 1983)} \\
& \log (P/\text{mmHg}) = 5.65204 – 648.629/(154.683 + t/°C); \text{ temp range 20–70°C (Antoine eq., Dean 1985, 1992)} \\
& 533.0 \text{ (Howard et al. 1986)} \\
& 1030 \text{ (20°C, Riddick et al. 1986)} \\
& 581.7 \text{ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)} \\
& \log (P/\text{kPa}) = 6.93296 – 1827.9/(-43.15 + T/K); \text{ temp range 341–414 K (Antoine eq., Stephenson & Malanowski } \text{1987)} \\
& 533, 12530 \text{ (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)} \\
& \log (P/\text{mmHg}) = 23.0607 – 3.1347 \times 10^3/(T/K) – 4.8813 \log (T/K) + 4.369 \times 10^{-5}/(T/K) – 4.9161 \times 10^{-13}(T/K)^2; \text{ temp range 287–615 K (vapor pressure eq., Yaws 1994)} \\
\text{Henry’s Law Constant (Pa·m}^3\text{/mol): } & 0.042 \text{ (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)}
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 0.43 (Leo et al. 1971)
- 0.31, 0.43 (calculated, Verschueren 1983)
- 0.35 (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, $t_{1/2}$:

Volatile:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.5–23.8$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24–168$ h, based on unacclimated aqueous screening test data (Dore et al. 1975; Sasaki 1978; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672–4320$ h, based on unacclimated anaerobic reactor test data (Chou et al. 1979; selected, Howard et al. 1991)

$K_{OC}$ (aerobic) $= 1$ d, $K_{OC}$ (anaerobic) $= 28$ d in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.5–23.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991); atmospheric transformation lifetime was estimated to be $< 1$ d (Kelly et al. 1994).

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

$K_{OC}$ (aerobic) $= 1$ d, $K_{OC}$ (anaerobic) $= 28$ d in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 48–4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (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:
13.1.1.11 Chloroacetic acid

\[
\text{Cl} - O - \text{Cl}
\]

Common Name: Chloroacetic acid
Synonym:
Chemical Name: chloroacetic acid (α or β)
CAS Registry No: 79-11-8
Molecular Formula: C₂H₃ClO₂, ClCH₂COOH
Molecular Weight: 94.497

Melting Point (°C):
- 61.2 (α, Stull 1947; Yalkowsky & Valvani 1980)
- 56.0 (β, Yalkowsky & Valvani 1980)
- 56–63 (Weast 1982–83; Dean 1985)
- 63 (Lide 2003)

Boiling Point (°C):
- 189.3 (Lide 2003)

Density (g/cm³ at 20°C):
- 1.4043 (40°C, Weast 1982–83)

Molar Volume (cm³/mol):
- 68.8 (63°C, Stephenson & Malanowski 1987)
- 89.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
- 2.85 (Weast 1982–83)

Enthalpy of Fusion, ΔHₜₜ (kJ/mol):
Entropy of Fusion, ΔSₜₜ (J/mol K):
- 56 (estimated, Yalkowsky & Valvani 1980)
- 36.73, 42.22 (observed for α, observed for β, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔSₜₜ = 56 J/mol K), F: 0.424 (mp at 63°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 120835 (α, calculated-ΔSₜₜ and mp, calculated-mp, Yalkowsky & Valvani 1980)
- 107200 (β, calculated-ΔSₜₜ and mp, calculated-mp, Yalkowsky & Valvani 1980)
- 109000 (shake flask-titrimetric assay, Bowden et al. 1998)

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):
- 39.70* (extrapolated-regression of tabulated data, temp range 43.0–189.5°C, Stull 1947)
- log (P/mmHg) = 8.28534 – 2263.7/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
- 6301* (112.8°C, ebulliometry, measured range 112.8–187.55°C, Dreisbach & Shrader 1949)
- 4141* (104.47°C, ebulliometry, measured range 104.47–190.27°C, McDonald et al. 1959)
- log (P/mmHg) = 7.56597 – 1733.96/(180.996 + t/°C); temp range: 104–190°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)
- log (P/mmHg) = [-0.2185 × 13134.5/(T/K)] + 9.099371; temp range 43–189°C (Antoine eq., Weast 1972–73)
- 18.52, 12.9 (extrapolated-Antoine eq., Boublik et al. 1984)
- log (P/kPa) = 6.67559 – 1723.714/(180.01 + t/°C); temp range 104–190.27°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) = 6.29612 – 1468.443/(154.397 + t/°C); temp range 123.19–187.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 18.52 (extrapolated-Antoine eq., Dean 1985)
- log (P/mmHg) = 7.55016 – 1723.365/(179.98 + t/°C); temp range 104–190°C (Antoine eq., Dean 1985, 1992)
- 8.51, 11.5 (extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.69087 - 1733.96/(–92.154 + T/K); temp range 336–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.67975 - 1727.293/(–97.742 + T/K); temp range 377–464 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/mmHg) = 42.6726 - 4.597 × 10³/(T/K) – 11.348·log (T/K) – 2.8515 × 10⁻¹⁰·(T/K)²; temp range 333–686 K (vapor pressure eq., Yaws 1994)

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

0.000938 (partial pressure equilibrium, Bowden et al. 1998)

ln [KH’/(mol kg⁻¹ atm⁻¹)] = –21.087 + 9742.6/(T/K), temp range 5–35°C (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_AW = 7.343 – 4104/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_ow:

0.22 (shake flask, Hansch & Leo 1987; recommended, Hansch et al. 1995)
0.22 (recommended, Sangster 1993)
0.22 (calculated-fragment const. with correction factors in multiCASE program, Dambrosky et al. 2001)

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: aqueous photolysis t½ = 1900–19000 h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991);
atmospheric photolysis t½ = 1900–19000 h, based on estimated aqueous photolysis half-life (Howard et al. 1991);
photocatalyzed mineralization by the presence of TiO₂ with the rate of 5.5 ppm/min per gram of catalyst (Ollis 1985).

Hydrolysis: first-order hydrolysis t½ = 23000 h, based on losses in dark control tests during photolysis experiments (Draper & Crosby 1983; quoted, Howard et al. 1991).

Oxidation: photooxidation t½ = 230–2300 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic t½ = 24–168 h, based on river die-away tests using radio-labeled material (Boethling & Alexander 1979; quoted, Howard et al. 1991); aqueous anaerobic t½ = 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: photooxidation t½ = 230–2300 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 5 d (Kelly et al. 1994).

Surface water: aqueous photolysis t½ = 1900–19000 h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991); t½ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).


Sediment:

Soil: t½ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
TABLE 13.1.1.11.1
Reported vapor pressures of chloroacetic acid at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

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

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

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<tr>
<th>Summary of literature data</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>ebulliometry</th>
<th>McDonald et al. 1959</th>
<th>ebullimetry</th>
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<td>169.0</td>
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<td>189.5</td>
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<td>62.65</td>
<td>eq. 2 P/mmHg</td>
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<tr>
<td>mp/°C</td>
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<tr>
<td>b.p. = 189.3 °C</td>
<td>m.p. = 63 °C</td>
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</table>

FIGURE 13.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for chloroacetic acid.
13.1.1.12 Dichloroacetic acid

Common Name: Dichloroacetic acid
Synonym: dichloroethanoic acid
Chemical Name: dichloroacetic acid
CAS Registry No: 79-43-6
Molecular Formula: C₂H₂Cl₂O₂, Cl₂CHCOOH
Molecular Weight: 128.942
Melting Point (°C):
13.5 (Lide 2003)
Boiling Point (°C):
194.0 (Weast 1982–83; Verschueren 1983; Lide 2003)
Density (g/cm³ at 20°C):
1.5634 (Weast 1982–83)
1.5630 (Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
82.50 (20°C, calculated-density, Stephenson & Malanowski 1987)
110.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
1.26 (Dean 1985)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
miscible (Dean 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
37.94* (extrapolated-regression of tabulated data, temp range 44–194.4°C, Stull 1947)
133.3 (44°C, Stull 1947; quoted, Verschueren 1983)
log (P/mmHg) = [–0.2185 × 12952.9/(T/K)] + 8.946605; temp range 44–194.4°C (Antoine eq., Weast 1972–73)
34.3 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 7.47122 – 2385.6/(–31.197 + T/K), temp range 317–468 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –7.2806 – 3.3706 × 10³/(T/K) + 9.3771·log (T/K) – 2.0832 × 10⁻²·(T/K)²; temp range 287–686 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.00085 (partial pressure equilibrium, Bowden et al. 1998)
ln [(K_H/ (mol kg⁻¹ atm⁻¹)] = −15.1776 + 8010.6/(T/K); temp range 5–35°C (partial pressure equilibrium measurements, Bowden et al. 1998)
0.000536 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 4.776 – 3352/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log K_{OW}:
0.92 (shake flask, Log P Database, Hansch & Leo 1987)
0.92 (recommended, Sangster 1993)
0.92 (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, \( t_{1/2} \):

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of TiO\(_2\) with the rate of 8.5 ppm/min per gram catalyst (Ollis 1985).

Half-Lives in the Environment:

### TABLE 13.1.12.1
Reported vapor pressures of dichloroacetic acid at various temperatures

<table>
<thead>
<tr>
<th>( T/\degree C )</th>
<th>( P/Pa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>44.0</td>
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<tr>
<td>69.8</td>
<td>666.6</td>
</tr>
<tr>
<td>82.6</td>
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<tr>
<td>96.3</td>
<td>2666</td>
</tr>
<tr>
<td>111.8</td>
<td>5333</td>
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<td>121.5</td>
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<td>152.3</td>
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<td>173.7</td>
<td>53329</td>
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<tr>
<td>194.4</td>
<td>101325</td>
</tr>
</tbody>
</table>

mp/\( \degree C \) 9.7

**FIGURE 13.1.12.1** Logarithm of vapor pressure versus reciprocal temperature for dichloroacetic acid.

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### 13.1.1.13 Trichloroacetic acid

![Chemical Structure](image)

**Common Name:** Trichloroacetic acid  
**Synonym:** TCA  
**Chemical Name:** trichloroacetic acid (α or β)  
**CAS Registry No:** 76-03-9  
**Molecular Formula:** Cl₃C(OH)  
**Molecular Weight:** 163.39  
**Melting Point (°C):**  
- 59.2 (Lide 2003)  
**Boiling Point (°C):**  
- 196.5 (Lide 2003)  
**Density (g/cm³ at 20°C):**  
- 1.620 (25°C, Weast 1982–83)  
**Molar Volume (cm³/mol):**  
- 100.3 (61°C, Stephenson & Malanowski 1987)  
- 131.1 (calculated-Le Bas method at normal boiling point)  
**Dissociation Constant, pKₐ:**  
- 0.70 (Weast 1982–83)  
- 0.52 (Dean 1985)  
**Enthalpy of Fusion, ΔHₘₙ (kJ/mol):**  
17.78, 56 (observed, estimated, Yalkowsky & Valvani 1980)  
**Entropy of Fusion, ΔSₘₙ (J/mol K):**  
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F: 0.462 (mp at 59.2°C)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
- 114550 (calculated-ΔSₘₙ and mp, Yalkowsky & Valvani 1980)  
- 191860 (calculated-mp, Yalkowsky & Valvani 1980)  
- 13000 (Verschueren 1983)  
- 1200000 (120 in 100 parts solvent, Dean 1985)  
- 383800 (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):**  
- 21.88* (extrapolated-regression of tabulated data, temp range 51–195.6°C, Stull 1947)  
- 4620* (112.62°C, ebulliometry, measured range 112.62–197.93°C, McDonald et al. 1959)  
- log (P/mmHg) = 7.31057 – 1618.97/(167.882 + t/°C); temp range 112.6–197.94°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)  
- log (P/mmHg) = [–0.2185 × 13817.0/(T/K)] + 9.341430; temp range 51–195.6°C (Antoine eq., Weast 1972–73)  
- 10.63 (extrapolated-Antoine eq., Boublik et al. 1984)  
- log (P/kPa) = 6.4026 – 1597.434/(165.711 + t/°C); temp range 112.6–197.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
- 66.14 (extrapolated-Antoine eq., Dean 1985)  
- log (P/mmHg) = 7.2730 – 1594.3/(165.4 + t/°C); temp range 112–198°C (Antoine eq., Dean 1985, 1992)  
- 133.3 (Howard et al. 1986; quoted, Banerjee et al. 1990)  
- 11.01 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
- log (P/kPa) = 6.43547 – 1618.97/(–105.268 + T/K); temp range 326–473 K (Antoine eq., Stephenson & Malanowski 1987)  
- 133.3, 491 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)  
- log (P/mmHg) = 63.4449 – 3.6769 × 10⁻³(T/K) – 21.13·log (T/K) + 1.0777 × 10⁻²·(T/K) + 4.8481 × 10⁻¹²·(T/K)²; temp range 258–491 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):

0.000137 (partial pressure equilibrium, Bowden et al. 1998)

\[ \ln \left[ \frac{K_H}{(mol \cdot kg^{-1} \cdot atm^{-1})} \right] = -17.836 + \frac{8660.09}{(T/K)}; \text{ temp range 5–35°C (partial pressure equilibrium measurements, Bowden et al. 1998)} \]

0.000834 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

\[ \log K_{AW} = 5.931 - \frac{3634}{(T/K)} \] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.33 (shake flask, Log P Database, Hansch & Leo 1987)
1.33 (recommended, Sangster 1993)
1.33 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, \( BCF \):

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

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

Volatilization:

Photolysis: no photocatalyzed mineralization by the presence of TiO₂ as compared to both dichloroacetic acid and trichloroacetic acid (Ollis 1985).

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 13.1.1.13.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of trichloroacetic acid at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>( \log P = A - B/(T/K) ) (1)</th>
<th>( \ln P = A - B/(T/K) ) (1a)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \log (P/mmHg) = A - B/(C + t/°C) ) (2)</td>
<td>( \ln P = A - B/(C + t/°C) ) (2a)</td>
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<tr>
<td></td>
<td>( \log (P/Pa) = A - B/(C + T/K) ) (3)</td>
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<td></td>
<td>( \log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K) ) (4)</td>
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</table>

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>McDonald et al. 1959</th>
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<tr>
<td>( t/°C )</td>
<td>( P/Pa )</td>
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<td>57.0 ( mp/°C )</td>
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FIGURE 13.1.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for trichloroacetic acid.
13.1.2 AROMATIC ACIDS

13.1.2.1 Benzoic acid

Common Name: Benzoic acid
Synonym:
Chemical Name: benzoic acid
CAS Registry No: 65-85-0
Molecular Formula: C₇H₆O₂, C₆H₅COOH
Molecular Weight: 122.122
Melting Point (°C):
122.35 (Lide 2003)
Boiling Point (°C):
249.2 (Lide 2003)
Density (g/cm³ at 20°C):
1.2659 (15°C, Weast 1982–83)
1.0800 (Dean 1985)
Molar Volume (cm³/mol):
113.6 (130°C, Stephenson & Malanowski 1987)
134.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
4.20 (McDaniel & Brown 1958)
4.33 ± 0.02, 4.38 ± 0.03 (HPLC, Unger et al. 1978)
4.08 (shake flask-TN, Clarke 1984)
4.05 ± 0.01 (equilibrium titration, Clarke & Cahoon 1987)
4.204 (Dean 1985; Lee et al. 1993)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
69.2 (395.2 K, de Kruif & Block 1982)
Enthalpy of Sublimation, ΔHₛₜₜₜ (kJ/mol):
94.5 (25°C, average value, Malaspina et al. 1973)
90.6 (Colomina et al. 1982)
90.51 (Ribeiro da Silva et al. 1995)
89.71 (Li et al. 2002)
90.1 (Li et al. 2004)
Enthalpy of Fusion, ΔHₕₜ (kJ/mol):
18.0 (Tsonopoulos & Prausnitz 1971)
18.2 (395.2 K, de Kruif & Block 1982)
Entropy of Fusion, ΔSₕₜ (J/mol K):
45.61 (Tsonopoulos & Prausnitz 1971)
43.81 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔSₕₜ = 56 J/mol K), F: 0.111 (mp at 122.35°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):
3340* (24.6°C, shake flask-synthetic method, Ward & Cooper 1930)
3298* (shake flask-thermostatic and synthetic methods, measured range 25–88.6°C, Morrision 1944)
4200 (shake flask-liquid scintillation counting, Lu & Metcalf 1975)
3600 (shake flask-UV, Yalkowsky et al. 1983)
3416* (shake flask-weight titration, measured temp range 5–65°C, Strong et al. 1989)
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):

- **799.9* (122.2°C, static method-manometer, measured range 122.2–249.0°C, Kahlbaum 1898)**
- **6.893* (60.1°C, isoteniscope method, measured range 60.1–247°C, Klosky et al. 1927)**
  - \( \log (P/\text{mmHg}) = 11.956 - 4409/(T/K) \); temp range 61–121°C (solid, isoteniscope, Klosky et al. 1927)
  - \( \log (P/\text{mmHg}) = 30.172 - 4714/(T/K) - 6.720 \cdot \log (T/K) \); temp range 128–247°C (liquid, isoteniscope, Klosky et al. 1927)

- **0.840* (extrapolated-regression of tabulated data, temp range 96–227°C, Stull 1947)**

- **12.35* (70.48°C, transpiration method, measured range 70.48–114.11°C, Davies & Jones 1954)**
  - \( \log (P/\text{mmHg}) = 12.45 - 4605/(T/K) \); temp range 344.4–393.8 K (isoteniscope method, Sachinidis & Hill 1980)

- **0.160* (96.05°C, Knudsen effusion weight-loss method, fitted to Antoine eq., measured range 65.05–110.25°C, Malaspina et al. 1973)**

- **0.108* (effusion method, measured range 25–70.5°C, DePablo 1976)**

- **16.8* (71.25°C, isoteniscope method, measured range 44.4–393.8 K, Sachinidis & Hill 1980)**
  - \( \log (P/\text{mmHg}) = 12.45 - 4605/(T/K) \); temp range 344.4–393.8 K (isoteniscope method, Sachinidis & Hill 1980)

- **0.112* (20°C, gas saturation method, vapor pressure balance, OECD 1981)**

- **0.105* (diaphragm manometer/torsion mass-loss effusion, extrapolated from measured range 316–391 K, de Kruif & Block 1982)**

- **0.0907 (20°C, evaporation method, Gückel et al. 1982)**

- **0.050* (20°C, gas saturation method, calculated-P/C, calculated-bond contribution, Meylan & Howard 1991)**

- **0.070* (20°C, gas saturation method, vapor pressure balance, OECD 1981)**

- **0.105 (20°C, gas saturation method, vapor pressure balance, OECD 1981)**

- **0.109 ± 0.005 (20°C, gas saturation-HPLC/UV, Sonnefeld et al. 1983)**

- **0.772 (liquid P L, extrapolated-Antoine eq., Dean 1989)**

- **0.840* (28°C, static method-manometer, measured range 122.2–249.0°C, Kahlbaum 1898)**

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

- **0.00709 (Howard 1989)**
- **0.00575; 0.0110 (calculated-P/C, calculated-bond contribution, Meylan & Howard 1991)**
- **0.00415 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)**
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 1.87 (shake flask-UV, Fujita et al. 1964)
- 1.68 (shake flask-UV, Halmekoski & Hannikainen 1964)
- 1.85 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
- 2.03 (shake flask-LSC, Lu & Metcalf 1975)
- 1.78 ± 0.01, 1.77 ± 0.01 (HPLC-k′ correlation, Unger et al. 1978)
- 1.79 (RP-HPLC-k′ correlation, D’Amboise & Hanai 1982)
- 1.86, 1.87 (calculated-fragment const., Rekker 1978)
- 1.94 (RP-HPLC correlation, Hanai & Hubert 1982)
- 1.95 (HPLC-k′ correlation; Miyake & Terada 1982)
- 1.87 (microelectrometric titration, Clarke 1984)
- 2.18 ± 0.03, 2.03 (exptl.-ALPM, selected best lit. value, Garst & Wilson 1984)
- 1.44, 1.87 (HPLC-k′ correlation, Haky & Young 1984)
- 1.88 (shake flask-UV at pH 0.5, Nishimura et al. 1985)
- 1.97 (microelectrometric titration, Clarke & Cahoon 1987)
- 1.94 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.93 (HPLC-k′ correlation, Miyake et al. 1987)
- 1.88 (CPC, Berthod et al. 1988)
- 1.85 ± 0.04 (“Filter Chamber”-UV, Hersey et al. 1989)
- 1.87 (recommended, Sangster 1989, 1993)
- 1.88 (back flashing-CPC centrifugal partition chromatography, Menges et al. 1990)
- 1.87 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

- 1.32, 2.00, 2.14 (fish, algae, mosquito, Lu & Metcalf 1975)
- 3.26, 3.45 (daphnia, snail, Lu & Metcalf 1975)
- 0.48 (algae Chlorella fusca, wet wt. basis, Geyer et al. 1984)
- 1.43 (algae Chlorella fusca, calculated-$K_{OW}$, Geyer et al. 1984)
- < 1.0 (golden ide, Freitag et al. 1985)
- < 1.0 (algae, Freitag et al. 1985)
- 3.11 (activated sludge, Freitag et al. 1985)
- 1.15 (trout muscle, calculated-$K_{OW}$, Branson 1978)

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

- 1.26; 1.86; 0.602 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 1.50 (soil, quoted exptl., Meylan et al. 1992)
- 1.16 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 1.50 (soil, calculated-MCI $^{1}\chi$, Sabljic et al. 1995)

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

Volatilization: rate of evaporation $k = 1.89 \times 10^{-8}$ mol cm$^{-2}$ h$^{-1}$ at 20°C determined by evaporation method (Gückel et al. 1982).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.0$ d, based on estimated vapor-phase reaction with hydroxyl radical in air (Howard 1989).

Hydrolysis: $k = 4.3 \times 10^{9}$ L mol$^{-1}$ s$^{-1}$ for reactions of hydroxyl radical in aqueous solution (Buxton et al. 1986)

$k = 1.15 \times 10^{13}$ M$^{-1}$ h$^{-1}$ (Mabury & Crosby 1996);

$k$ (exptl) = $1.2 \times 10^{13}$ M$^{-1}$ h$^{-1}$ for reaction with hydroxy radical (Armbrust 2000)

Biodegradation: completely degraded by a soil microflora after 24 h (Alexander & Lustigman 1966; quoted, Verschuuren 1983);

completely degraded for 16 mg/L concn. within one day by soil and by wastewater (Haller 1978);
Carboxylic Acids

$t_{1/2} \sim 0.2–3.6 \text{ d if released into water, should readily biodegrade (Howard 1989);}$

average $k(\text{exptl}) = 0.11533 \text{ h}^{-1}$ compared to group method predicted $k = 0.0993 \text{ h}^{-1}$ (nonlinear) and $k = 0.0263 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation: degradation $k = 6.84 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.0 \text{ d for reactions with photochemically produced hydroxyl radical (Howard 1989).}$

Surface water: if released into water, should readily biodegrade with an estimated $t_{1/2} = 0.2–3.6 \text{ d (Howard 1989).}$

Groundwater:

Sediment:

Soil:

Biota:

**TABLE 13.1.2.1.1**

Reported aqueous solubilities of benzoic acid at various temperatures

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**FIGURE 13.1.2.1.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benzoic acid.
### Table 13.1.2.1.2
Reported vapor pressures of benzoic acid at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

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

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

1. **Kahlbaum 1898**
   - Static method-manometer*
   - **Klosky et al. 1927**
     - Isoteniscope method
   - **Stull 1947**
     - Summary of literature data
   - **Davies & Jones 1954**
     - Knudsen effusion

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\*Complete list see ref.

\[ \Delta H_{\text{subl}}/(kJ/mol) = 91.42 \]

\[ \Delta H_{\text{subl}}/(kJ/mol) = 94.37 \]

\[ \Delta H_{\text{subl}}/(kJ/mol) = 94.37 \]

2. **Wiedemann 1971**
   - Knudsen effusion
   - **Malaspina et al. 1973**
     - Knudsen effusion
   - **Sachinidis & Hill 1980**
     - Isoteniscope-manometer
   - **OECD 1981**
     - Gas saturation/effusion

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3.

Colomina et al. 1982 | de Kruif & Block 1982 | Li et al. 2002 |
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FIGURE 13.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzoic acid.
13.1.2.2 2-Methyl benzoic acid (o-Toluic acid)

\[ \text{O}_2\text{N} \cdot \text{OH} \]

Common Name: o-Toluic acid
Synonym: 2-methyl benzoic acid
Chemical Name: o-toluic acid, 2-methyl benzoic acid
CAS Registry No: 118-90-1
Molecular Formula: C_{8}H_{8}O_{2}, CH_{3}C_{6}H_{4}COOH
Molecular Weight: 136.149
Melting Point (°C):
103.5 (Lide 2003)
Boiling Point (°C):
259 (Lide 2003)
Density (g/cm³ at 20°C):
1.062 (115°C, Weast 1982–83; Verschueren 1983)
Molar Volume (cm³/mol):
157.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
3.91 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)
3.91 (Weast 1982–83)
3.90 (Dean 1985)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
20.17 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
53.56 (Tsonopoulos & Prausnitz 1971)
53.5, 56 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 0.170 (mp at 103.5°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):
22300* (85.1°C, shake flask-residue volume, measured range 85.1–102.4°C, Sidgwick et al. 1915)
1185 (shake flask, Fühner 1924)
1162* (shake flask-weight titration, measured range 5–65°C, Strong et al. 1989)
1074* (shake flask-UV, Sugunan & Thomas 1993)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
log \( (P/\text{mmHg}) = -35.8816 - 3.2354 \times 10^{1}/(T/K) + 21.133 \log (T/K) - 3.0165 \times 10^{-2}(T/K) + 1.1587 \times 10^{-5}(T/K)^{2}; \)
temp range 377–751 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
2.18 (shake flask-UV, Tomida et al. 1978)
2.81 (Scherrer & Howard 1979)
2.46 (shake flask at pH 1, Hansch & Leo 1987)
2.27 (shake flask-UV at pH 2, Da et al. 1992)
2.46 (recommended, Sangster 1993)
2.46 (recommended, pH 1, Hansch et al. 1995)
1.72 (RP-HPLC-RT correlation on short ODP column, pH 2, Donovan & Pescatore 2002)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants or Half-Lives:
- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:

**TABLE 13.1.2.2.1**

Reported aqueous solubilities of 2-methylbenzoic acid (o-toluic acid) at various temperatures

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<thead>
<tr>
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<th>t/°C</th>
<th>S/g·m⁻³</th>
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<th>S/g·m⁻³</th>
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<tr>
<td>mp</td>
<td>102.4°C</td>
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FIGURE 13.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methylbenzoic acid.
13.1.2.3 3-Methyl benzoic acid (m-Toluic acid)

Common Name: m-Toluic acid
Synonym: 3-methyl benzoic acid
Chemical Name: m-toluic acid, 3-methyl benzoic acid
CAS Registry No: 99-04-7
Molecular Formula: C₈H₈O₂, CH₃C₆H₄COOH
Molecular Weight: 136.149
Melting Point (°C):
109.9 (Lide 2003)
Boiling Point (°C):
263.0 (sublimation, Weast 1982–83)
Density (g/cm³ at 20°C):
1.054 (112°C, Weast 1982–83; Verschueren 1983)
Molar Volume (cm³/mol):
129.2 (112°C, Stephenson & Malanowski 1987)
157.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
4.270 (Weast 1982–83)
4.269 (Dean 1985)
4.220 (Sangster 1993)
Enthalpy of Fusion, ΔHₕus (kJ/mol):
15.73 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔSₕus (J/mol K):
10.96 (Tsonopoulos & Prausnitz 1971)
41.17, 56 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔSₕus = 56 J/mol K), F: 0.147 (mp at 109.9°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):
11600* (80°C, shake flask-residue volume, measured range 80–110.5°C, Sidgwick et al. 1915)
982 (shake flask-residue volume method, Fühner 1924)
1700 (20–25°C, shake flask-GC, Urano et al. 1982)
872* (shake flask-weight titration, measured range 5–65°C, Strong et al. 1989)
1246* (shake flask-UV, Sugunan & Thomas 1993)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
log (Pₛ/kPa) = 8.1472 – 3280.8/(T/K), temp range 473–533 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₐow:
2.37 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
2.43 (HPLC-′k correlation, Miyake & Terada 1982)
2.41 (shake flask-AS, Miyake et al. 1987)
2.39 (centrifugal partition chromatography CPC, Terada et al. 1987)
2.44; 2.47 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
2.38 (shake flask-UV at pH 2, Da et al. 1992)
2.37 (recommended, Sangster 1993)
2.37 (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:
- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biotransformation:
  - Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

### TABLE 13.1.2.3.1
Reported aqueous solubilities of 3-methylbenzoic acid (m-toluic acid) at various temperatures

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<thead>
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<th>Strong et al. 1989</th>
<th>Sugunan &amp; Thomas 1993</th>
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<td>shake flask-titration</td>
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<td>$t/°C$</td>
<td>$S/g\cdot m^{-3}$</td>
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<td>621</td>
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</table>

$\Delta H_{sol}/(kJ\cdot mol^{-1}) = 26.15$ at 25°C

critical solution temp 162.2°C
triple point 142.0°C
mp 110.5°C
FIGURE 13.1.2.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-methylbenzoic acid ($m$-toluic acid).

- Critical solution temp. = 162.2 °C
- m.p. = 109.9 °C

Legend:
- Diamond: Sidgwick et al. 1915
- Triangle: Strong et al. 1989
- Square: Sugunan & Thomas 1993
13.1.2.4 4-Methyl benzoic acid (p-Toluic acid)

CAS Registry No: 99-94-5
Molecular Weight: 136.149

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

Dissociation Constant, pKₐ:
4.37, 4.30 ± 0.09 (quoted, HPLC, Unger et al. 1978)
4.37, 4.41 ± 0.01 (quoted, HPLC, Unger et al. 1978)
4.36 (Weast 1982–83)
4.37, 4.26 (quoted, shake flask-TN, Clarke 1984)
4.362 (Dean 1985)
4.39 (Sangster 1993)

Enthalpy of Fusion, ΔHₛᵤ₃ (kJ/mol):
22.72 (Tsonopoulos & Prausnitz 1971)
23.81 (differential scanning calorimetry, Li et al. 2001)

Entropy of Fusion, ΔSₛᵤ₃ (J/mol K):
50.21 (Tsonopoulos & Prausnitz 1971)
50.21, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔSₛᵤ₃ = 56 J/mol K), F: 0.0304 (mp at 179.6°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):
11600* (100, shake flask-residue volume, measured range 100–176.8°C, Sidgwick et al. 1915)
383 (selected, Tsonopoulos & Prausnitz 1971)
343* (shake flask-weight titration, measured range 5–65°C, Strong et al. 1989)
331* (shake flask-UV, Sugunan & Thomas 1993)
378.5* (shake flask-titration, measured range 278.15–343.15 K, Apelblat & Manzurola 1999)
ln [m/(mol kg⁻¹)] = –264.605 – 9059.53/(T/K) + 40.069·ln (T/K); temp range 278–343K (shake flask-titration, Apelblat & Manzurola 1999)
371* (shake flask-laser monitoring observation technique, measured range 288.35–370.95 K, Li et al. 2001)
393* (26.4°C, synthetic method-laser technique, measured range 290.25–348.45 K, Chen & Ma 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
30.93* (95.20°C, Knudsen effusion, measured range 95.2–134.96°C (Davies & Jones 1954)
log (P/mmHg) = 128585 – 4968.7/(T/K); temp range 95.2–134.96°C (Knudsen effusion, Davies & Jones 1954)
log (P/mmHg) = –67.6587 – 2.2339 × 10¹/(T/K) + 33.347·log (T/K) – 3.7709 × 10⁻³/(T/K) + 1.313 × 10⁻⁵·(T/K)²; temp range 453–773 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 2.27 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)
- 2.22 ± 0.02, 2.26 ± 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.36 (shake flask-UV at pH 2, Ezumi & Kubota 1980)
- 2.43 (calculated-HPLC-k' correlation, Miyake & Terada 1982)
- 2.34 (electrometric titration, Clarke 1984)
- 2.67 (HPLC-RT correlation, Garst 1984)
- 2.66 (centrifugal partition chromatography CPC, Terada et al. 1987)
- 2.38; 2.41 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
- 2.35 (HPLC-RT correlation, Jenke et al. 1990)
- 2.26 (shake flask-UV at pH 2, Da et al. 1992)
- 2.34 (recommended, Sangster 1994)
- 2.27 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log $BCF$:

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

- 2.15, 1.15, 1.30 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.77 (soil, quoted exptl., Meylan et al. 1992)
- 1.37 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:


Biotransformation:

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

Half-Lives in the Environment:

### TABLE 13.1.2.4.1
Reported aqueous solubilities of 4-methylbenzoic acid (p-toluic) acid at various temperatures

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<tbody>
<tr>
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<td>shake flask-titration</td>
<td>shake flask-UV</td>
<td>shake flask-titration</td>
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<td>t/°C</td>
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<td>S/g·m⁻³</td>
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<td>&amp; &amp;</td>
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<td>34.7</td>
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<td>87.7</td>
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</table>

(Continued)
### TABLE 13.1.2.4.1  (Continued)

<table>
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<tr>
<th>Li et al. 2001</th>
<th>Chen &amp; Ma 2004</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake flask-laser monitor</td>
<td>synthetic method</td>
</tr>
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<td>( t / ^{\circ} C )</td>
<td>( S / g \cdot m^{-3} )</td>
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<td>95.5</td>
<td>5204</td>
</tr>
<tr>
<td>97.8</td>
<td>5726</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{ fus}} / (kJ \ mol^{-1}) = 23.81 \]

### FIGURE 13.1.2.4.1

Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for 4-methylbenzoic acid (\( p\)-toluic acid).

4-Methylbenzoic acid (\( p\)-Toluic acid): solubility vs. \( 1/T \)

- Sidgwick et al. 1915
- Strong et al. 1989
- Sugunan & Thomas 1993
- Apelblat & Marzuola 1999
- Li et al. 2001
- Chen & Ma 2004
Common Name: Phenylacetic acid
Synonym: phenylethanoic acid, α-toluic acid, benzeneacetic acid
Chemical Name: phenylacetic acid
CAS Registry No: 103-82-2
Molecular Formula: C₈H₈O₂, C₆H₅CH₂COOH
Molecular Weight: 136.149
Melting Point (°C):

76.5 (Lide 2003)

Boiling Point (°C):

265.5 (Stull 1947; Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):

1.081 (Verschueren 1983)
Molar Volume (cm³/mol):

124.8 (77°C, Stephenson & Malanowski 1987)
157.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:

4.28 (18°C, Weast 1982–83)
4.31 (Sangster 1989)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):

17.11 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔSₘₚ (J/mol K):

48.95 (Tsonopoulos & Prausnitz 1971)
41.42, 56 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F: 0.312 (mp at 76.5°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):

17700* (thermostatic and synthetic methods, measured range 25–86.7°C, Morrison 1944)
16600 (20°C, Hodgman 1952)
17790 (selected, Tsonopoulos & Prausnitz 1971)
16600 (20°C, quoted, Verschueren 1983)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.835 (extrapolated-regression of tabulated data, temp range 97–265°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 15568.7/(T/K)] + 9.206178; temp range 97–265.5°C (Antoine eq., Weast 1972–73)
0.827 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P₁/kPa) = 8.00148 – 3144.95/(–14.408 + T/K); temp range 370–539 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):

0.0056 (calculated-P/C)
Octanol/Water Partition Coefficient, log Kₐw:

1.41 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971)
1.41 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
1.51 (shake flask-UV, Yaguzhinskii et al. 1973)
1.94 (RP-LC-RT correlation, Hanai & Hubert 1982)
1.45 (shake flask-UV at pH 3.5, Kuchar et al. 1982)
1.95 ± 0.04; 1.51 (exptl.-ALPM, selected best lit. value, Garst 1984)
1.41 (recommended, Sangster 1989, 1993)
1.34 ± 0.14, 1.07 ± 0.49 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
1.41 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:
1.49, 1.42, 1.45 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
1.45 (soil, quoted exptl., Meylan et al. 1992)
1.42 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
1.45 (soil, quoted or calculated-QSAR MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_\frac{1}{2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

TABLE 13.1.2.5.1
Reported aqueous solubilities of phenylacetic acid at various temperatures:

<table>
<thead>
<tr>
<th>$t/^\circ$C</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>17700</td>
</tr>
<tr>
<td>35.0</td>
<td>26005</td>
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<td>39484</td>
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<td>83.0</td>
<td>83188</td>
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<tr>
<td>86.7</td>
<td>93399</td>
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</table>
FIGURE 13.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phenylacetic acid.
13.1.2.6 Phthalic acid

Common Name: Phthalic acid
Synonym: 1,2-benzene dicarboxylic acid, o-phthalic acid
Chemical Name: 1,2-benzene dicarboxylic acid, o-phthalic acid
CAS Registry No: 88-99-3
Molecular Formula: C₈H₆O₄, C₆H₄-1,2-(COOH)₂
Molecular Weight: 166.132
Melting Point (°C):
230 (dec., Lide 2003)
Boiling Point (°C):
Dec (Lide 2003)
Density (g/cm³ at 20°C):
1.593 (West 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
173.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
2.89, 5.51 (pK₁, pK₂, West 1982–83)
2.95, 5.408 (pK₁, pK₂, Dean 1985)
Enthalpy of Fusion, ΔHₛₒₜ (kJ/mol):
Entropy of Fusion, ΔSₛₒₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₛₒₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section)
7014* (shake flask-synthetic method, measured range 25–85°C, McMaster et al. 1921):
7160* (25.8°C, shake flask-synthetic method, measured range 25.8–113.8°C, Ward & Cooper 1930)
5400 (14°C, Verschueren 1983)
6300 (Dean 1985)
7024* (shake flask, measured range 283.65–338.15 K, Apelblat & Manzurola 1989)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
\[ \log (P/mmHg) = -90.3221 - 3.2214 \times 10^3/(T/K) + 44.109 \log (T/K) - 5.0056 \times 10^{-2} (T/K) + 1.6895 \times 10^{-5} (T/K)^2; \]
temp range 464–800 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log Kᵪₒₜ:
0.79 (shake flask-UV, Tomida et al. 1978)
0.15 (electrometric titration, Freese et al. 1979)
0.73 (shake flask at pH 1, Log P Database, Hansch & Leo 1987)
0.71 (30°C, shake flask-UV at pH 1, Patronkey & Pflegel 1992)
0.73 (recommended, Sangster 1993)
0.73 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF:
Carboxylic Acids 2749

Sorption Partition Coefficient, $\log K_{OC}$:
- 0.301, 1.49, 0.301 (sediment, Podzol soil, Alfidol soil, von Oepen et al. 1991)
- 1.07 (soil, quoted exp., Meylan et al. 1992)
- 1.87 (soil, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
- 1.07 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)

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

- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
- Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
  - average rate of biodegradation 78.4 mg COD g$^{-1}$·h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air:
- Surface water:
- Groundwater:
- Sediment:
  - Soil: degradation $t_{1/2} = 2$ d in initial phase, $t_{1/2} = 15$ d in late phase in sludge-amended soil (Roslev et al. 1998)
  - Biota:

### TABLE 13.1.2.6.1
Reported aqueous solubilities of o-phthalic acid at various temperatures

<table>
<thead>
<tr>
<th>Temperature</th>
<th>McMaster et al. 1921</th>
<th>Ward &amp; Cooper 1930</th>
<th>Apelblat &amp; Manzurola 1989</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
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<tr>
<td>25</td>
<td>7014</td>
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</tbody>
</table>

$\Delta H_{sol}/(kJ\ mol^{-1}) = 29.0$
FIGURE 13.1.2.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for phthalic acid.
13.1.2.7 2-Chlorobenzoic acid

\[
\begin{align*}
\text{Common Name:} & \quad \text{2-Chlorobenzoic acid} \\
\text{Synonym:} & \quad o\text{-chlorobenzoic acid} \\
\text{Chemical Name:} & \quad 2\text{-chlorobenzoic acid}, \quad o\text{-chlorobenzoic acid} \\
\text{CAS Registry No:} & \quad 118-91-2 \\
\text{Molecular Formula:} & \quad C_7H_5ClO_2, \quad ClC_6H_4COOH \\
\text{Molecular Weight:} & \quad 156.567 \\
\text{Melting Point (°C):} & \quad 140.2 \quad \text{\cite{Lide2003}} \\
\text{Boiling Point (°C):} & \quad \text{sublimation (Verschueren 1983; Lide 2003)} \\
\text{Density (g/cm}^3\text{ at 20°C):} & \quad 1.5440 \quad \text{\cite{Weast1982,Verschueren1983}} \\
\text{Molar Volume (cm}^3\text{/mol):} & \quad 101.4 \quad \text{\cite{Weast1982}} \\
\text{Dissociation Constant, pK}_a: & \quad 2.920 \quad \text{\cite{Mcdaniel1958,Pearce1968,Weast1982}} \\
\text{Enthalpy of Fusion, } \Delta H_{\text{ fus}} \text{ (kJ/mol):} & \quad 25.73 \quad \text{\cite{Tsonopoulos1971}} \\
\text{Entropy of Fusion, } \Delta S_{\text{ fus}} \text{ (J/mol K):} & \quad 62.34 \quad \text{\cite{Tsonopoulos1971}} \\
\text{Water Solubility (g/m}^3\text{ or mg/L at 25°C):} & \quad 2130 \quad \text{\cite{Osol1933}} \\
\text{Vapor Pressure (Pa at 25°C):} & \quad \log (P/mmHg) = -42.9847 -3.1867 \times 10^3/(T/K) + 23.694 \log (T/K) - 3.0284 \times 10^{-2} \times (T/K)^2; \quad \text{temp range 415–792 K (vapor pressure eq., Yaws 1994)} \\
\text{Henry’s Law Constant (Pa-m}^3\text{/mol at 25°C):} & \quad 1.98 \quad \text{\cite{Leo1971,Hansch1979}} \\
\text{Octanol/Water Partition Coefficient, } \log K_{\text{OW}}: & \quad 2.63, 2.56 \quad \text{\cite{Rekker1977}} \\
\end{align*}
\]
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, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biodegradation: decomposition by soil microflora: $t_{1/2} > 64$ d, biodegradation by waste water at pH 7.3 and 30°C, $t_{1/2} > 25$ d, and degradation by soil suspension at pH 7.3 and 30°C; $t_{1/2} = 7$–14 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); complete degradation of 16 mg/L by soil in 7–14 d (Haller 1978).
- Biotransformation:

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
13.1.2.8 3-Chlorobenzoic acid

Common Name: 3-Chlorobenzoic acid
Synonym: m-chlorobenzoic acid
Chemical Name: 3-chlorobenzoic acid, m-chlorobenzoic acid
CAS Registry No: 535-80-8
Molecular Formula: C₇H₅ClO₂, ClC₆H₄COOH
Molecular Weight: 156.567
Melting Point (°C):
  158 (Weast 1982–83; Verschueren 1983; Lide 2003)
Boiling Point (°C):
  sublimation (Weast 1982–83; Verschueren 1983; Lide 2003)
Density (g/cm³ at 20°C):
  1.4960 (25°C, Weast 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
  104.7 (25°C, calculated-density)
  155.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
  3.82 (Weast 1982–83)
  3.83 (Dean 1985)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
  23.85 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ∆S_fus (J/mol K):
  55.65 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F: 0.0496 (mp at 158°C)
Water Solubility (g/m³ or mg/L at 25°C):
  385 (Osol & Kilpatrick 1933)
  398 (selected, Tsonopoulos & Prausnitz 1971)
  400 (0°C, Verschueren 1983)
  400 (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:
  2.68 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979)
  2.65, 2.52 (calculated-fragment const., calculated-π const, Rekker 1977)
  0.89 (HPLC-RT correlation, Veith et al. 1979)
  2.57 (HPLC-K′ correlation, Miyake & Terada 1982)
  2.62 (centrifugal partition chromatography, Terada et al. 1987)
  2.51; 2.58 (shake flask at pH 1; HPLC-RT correlation, Wang et al. 1989)
  2.72 (shake flask-UV at pH 2, Da et al. 1992)
  2.60 (recommended, Sangster 1993)
  2.68 (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, \( t_{1/2} \):
- Volatilization:
  - Photolysis: direct aqueous photolysis \( k = 0.013 \pm 0.001 \text{ min}^{-1} \) with \( t_{1/2} = 55 \text{ min} \) (Stegeman et al. 1993).
- Oxidation:
- Hydrolysis:
  - Biodegradation: decomposed by soil microflora, \( t_{1/2} = 32 \text{ d} \) (Alexander & Lustigman 1966; quoted, Verschueren 1983);
  - complete degradation of 16 mg/L by soil and by wastewater in 7–14 d (Haller 1978).

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

Half-Lives in the Environment:
- Air:
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota:
13.1.2.9 4-Chlorobenzoic acid

Common Name: 4-Chlorobenzoic acid
Synonym: p-chlorobenzoic acid
Chemical Name: 4-chlorobenzoic acid, p-chlorobenzoic acid
CAS Registry No: 74-11-3
Molecular Formula: C₇H₅ClO₂, ClC₆H₄COOH
Molecular Weight: 156.567
Melting Point (°C):
243.0 (Weast 1982–83; Verschueren 1983; Lide 2003)
Boiling Point (°C):
sublimation (Verschueren 1983)
Density (g/cm³ at 20°C):
1.541 (24°C, Verschueren 1983)
Molar Volume (cm³/mol):
155.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
3.98 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)
3.98 (Weast 1982–83)
3.98, 3.85 (quoted, shake flask-TN, Clarke 1984)
3.986 (Dean 1985)
3.850 (Sangster 1993)
Enthalpy of Fusion, ΔHₚᵤₛ (kJ/mol):
32.26 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔSₚᵤₛ (J/mol K):
62.76 (Tsonopoulos & Prausnitz 1971)
62.9, 56 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔSₚᵤₛ = 56 J/mol K), F: 0.00726 (mp at 243°C)
Water Solubility (g/m³ or mg/L at 25°C):
68.0 (Osol & Kilpatrick 1933)
72.6 (selected, Tsonopoulos & Prausnitz 1971)
77.0 (Verschueren 1983)
200 (Dean 1985)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m²/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
2.65 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
2.65; 2.52 (calculated-fragment const., calculated-π const., Rekker 1977)
2.53; 2.65 (HPLC-k' correlation, Miyake & Terada 1982)
2.66 (electrometric titration, Clarke 1984)
2.65 (centrifugal partition chromatography, Terada et al. 1987)
2.60; 2.67 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
2.67 (HPLC-RT correlation, Wang et al. 1989)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:
- < 1.0, 1.80, 2.23 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- 1.80, 1.99 (alga *chlorella fusca*, wet wt. basis, calculated-$K_{OW}$, Geyer et al. 1984)
- < 1.0, 1.78, 2.23 (golden ide, algae, activated sludge, Freitag et al. 1985)

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

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation:
  - $k(aq.) \leq 0.15 \, M^{-1} \, s^{-1}$ for direct reaction with ozone in water at pH 2–6 and 22 ± 1°C, with $t_{1/2} \geq 3 \, d$ at pH 7 (Yao & Haag 1991).
- Hydrolysis:
- Biodegradation: decomposition by a soil microflora, $t_{1/2} = 64 \, d$; degradation by waste water or soil suspension at pH 7.3 and 30°C, $t_{1/2} > 25 \, d$ (quoted, Verschueren 1983).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air:
  - Surface water: $t_{1/2} \geq 3 \, d$ at pH 7 based on reaction rate with ozone in water (Yao & Haag 1991)
- Groundwater:
- Sediment:
- Soil:
- Biota:
13.1.2.10 Salicylic acid

Common Name: Salicylic acid
Synonym: 2-hydroxybenzoic acid, o-hydroxybenzoic acid
Chemical Name: salicylic acid, 2-hydroxybenzoic acid
CAS Registry No: 69-72-7
Molecular Formula: C7H6O3, HOC6H4COOH
Molecular Weight: 138.121
Melting Point (°C): 159.0 (Weast 1982–83; Lide 2003)
Boiling Point (°C): 256 (Verschueren 1983)
Density (g/cm³ at 20°C): 1.443 (Weast 1982–83; Verschueren 1983)
Molar Volume (cm³/mol): 95.7 (20°C, calculated-density)
147.4 (158.6°C, Stephenson & Malanowski 1987)
142.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
3.009 (Korman & La Mer 1936)
3.52 ± 0.03 (HPLC, Unger et al. 1978)
3.29 ± 0.03 (HPLC, Unger et al. 1978)
2.96 (equilibrium titration, Clarke & Cahoon 1987)
2.97 (Sangster 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: 0.0484 (mp at 159°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):
5570* (50°C, synthetic method, measured range 50–159°C, critical solution temp. 89.5°C, Sidgwick & Ewbank 1921)
1840* (20°C, Hodgman 1952; Verschueren 1983)
1550 (shake flasks-UV, Yalkowsky et al. 1983)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (113.7°C, summary of literature data, temp range 113.7–159°C, Stull 1947)
30.93* (95.20°C, transpiration method, measured range 95.2–134.96°C, Davies & Jones 1954)
log (P/mmHg) = 12.8585 – 4968.7/(T/K), temp range 70.48–114.11°C (transpiration, Davies & Jones 1954)
log (P/mmHg) = −0.2185 × 18920.7/(T/K) + 10.822961; temp range 113.7–256.0°C (Antoine eq., Weast 1972–73)
2.85 (70.5°C, effusion method, DePablo 1976)
0.0208 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 11.9834 – 4968.7/(T/K); temp range 368–408 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P/kPa) = 5.53812 – 1049.95/(-228.144 + T/K); temp range 445–504 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = 177.3858 – 1.2871 × 10^4/(T/K) – 56.301·log (T/K) – 1.6667 × 10^-7·(T/K)^2;
temp range 432–739 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
0.00144 (calculated-P/C)

Octanol/Water Partition Coefficient, log K_{ow}:
2.26 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1971)
2.21 (shake flask, unpublished result, Leo et al. 1971)
2.24 (shake flask, pH 2, Korenman 1975)
2.38 (shake flask-UV, Tomida et al. 1978)
2.00 ± 0.01, 2.18 ± 0.01 (HPLC-RT correlation, Unger et al. 1978)
2.26, 2.21, 2.24, 2.25, 0.95 (quoted lit. values; Hansch & Leo 1979)
1.90 (HPLC-RT correlation, Butte et al. 1981)
2.25 ± 0.03 (exptl.-ALPM, Garst & Wilson 1984)
1.13, 1.92 (HPLC-k’ correlation, Haky & Young 1984)
2.21 (shake flask-HPLC at pH 2, Bundgaard et al. 1986; Bundgaard & Nielsen 1988)
2.34 (electrometric titration, Clarke & Cahoon 1987)
2.24 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
1.08 (RP-TLC retention time correlation, Jack et al. 1988)
–0.78 (shake flask-UV, Kuban 1991)
2.64 (centrifugal partition chromatography, Ichmann et al. 1993)
2.26 (recommended, Sangster 1993)
–2.11 (recommended, pH 7.4, Hansch et al. 1995)
–1.70 (pH 7.0), –0.90 (pH 7.4); 2.26 (literature values; Hansch et al. 1995)
2.02 (shake flask-micro-volume liquid-liquid flow extraction system, Carlsson & Karlberg 2000)
–1.44 (shake flask, buffered with 20 mM phosphate buffer pH 7.4, Carlsson & Karlberg 2000)

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 constants k < 600 M^-1 s^-1 at pH 1.3–3, k = (30 ± 10) × 10^9 M^-1 s^-1 at pH 4–7 using 4 mM t-BuOH as scavenger for the reaction with ozone in water and 20–23°C (Hoigné & Bader 1983a);
rate constants k < 500 M^-1 s^-1 for protonated species, k = (2.8 ± 3) × 10^9 M^-1 s^-1 for non-protonated species for the reaction with ozone in water using 4 mM t-BuOH as scavenger at pH 1.5–7 and 20–23°C (Hoigné & Bader 1983b).

Hydrolysis:
Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); average rate of biodegradation 95.0 mg COD g^-1·h^-1 based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Biocorcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
TABLE 13.1.2.10.1
Reported aqueous solubilities of salicylic acid at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>T/K</th>
<th>S/g·m⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.0</td>
<td>5570</td>
<td>10</td>
<td>1310</td>
<td>283.15</td>
<td>1533</td>
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<td>80.0</td>
<td>20260</td>
<td>30</td>
<td>2610</td>
<td>307.15</td>
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<td>97.9</td>
<td>52700</td>
<td>40</td>
<td>3950</td>
<td>317.15</td>
<td>4393</td>
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<td>101.4</td>
<td>80200</td>
<td>50</td>
<td>5920</td>
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<td>105.6</td>
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<td>8640</td>
<td>320.15</td>
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<td>339.15</td>
<td>11433</td>
</tr>
</tbody>
</table>

Critical solution temp 89.5°C

ΔHsol/(kJ mol⁻¹) = 24.0
for temp range 288–313 K

FIGURE 13.1.2.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for salicylic acid.
TABLE 13.1.2.10.2
Reported vapor pressures of salicylic acid at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>113.7</td>
<td>133.3</td>
<td>136.0</td>
<td>666.6</td>
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<td>136.0</td>
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<td>146.2</td>
<td>100.49</td>
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<tr>
<td>182.0</td>
<td>13332</td>
<td>193.4</td>
<td>119.98</td>
</tr>
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<td>26664</td>
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<td>125.13</td>
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<td>210.0</td>
<td>101325</td>
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<td>134.96</td>
</tr>
<tr>
<td>230.5</td>
<td>53329</td>
<td>256.0</td>
<td>159</td>
</tr>
</tbody>
</table>

Knudsen effusion

mp/°C 159

\[ \Delta H_{subl} / (kJ mol^{-1}) = 95.144 \]

FIGURE 13.1.2.10.2 Logarithm of vapor pressure versus reciprocal temperature for salicylic acid.
13.1.2.11 2,4-Dichlorophenoxyacetic acid (2,4-D) (See also Chapter 17, Herbicides)

Common Name: 2,4-Dichlorophenoxyacetic acid
Synonym: 2,4-D
Chemical Name: 2,4-dichlorophenoxyacetic acid
CAS Registry No: 94-75-7
Molecular Formula: C₈H₆Cl₂O₃, Cl₂C₆H₃OCH₂COOH
Molecular Weight: 221.038

Melting Point (°C):
140.5 (Hartley & Kidd 1987; Howard 1991; Lide 2003)

Boiling Point (°C):
160 (at 0.4 mmHg, Dean 1985; Howard 1991)
215 (Neely & Blau 1985)

Density (g/cm³ at 30°C):
1.565 (Neely & Blau 1985)

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

Dissociation Constant, pKₐ:
2.77 (potentiometric, Nelson & Faust 1969)
2.87 (spectrophotometric, Cessna & Grover 1978)
2.80 (Reinert & Rogers 1984)
2.64–3.31 (Howard 1991)
2.80 (selected, Wauchope et al. 1992)
2.97 (Sangster 1993)

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: 0.0736 (mp at 140.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
522 (shake flask-UV, Leopold et al. 1960)
725 (Bailey & White et al. 1965)
725, 400, 900, 550 (review, Günther et al. 1968)
890 (Hamaker 1975)
900 (Kenaga 1980a,b; Kenaga & Goring 1980)
600 (20°C, Khan 1980)
470 (20–25°C, pH 5.6, Geyer et al. 1981)
620 (20°C, Kidd & Hartley 1987; Worthing 1983)
609 (Gerstl & Helling 1987)
682 (Yalkowsky et al. 1987; quoted, Howard 1991)
703 (Gustafson 1989)
900, 600, 890, 703, 1072 (quoted, Wauchope et al. 1992)
890 (20–25°C, selected, Wauchope et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated):
8.0 × 10⁻⁵ (Hamaker 1975)
0.180–1.69 (transpiration method, Spencer 1976)
53.0 (160°C, Kidd & Hartley 1983, 1987)
8.0 × 10⁻⁵ (recommended, Neely & Blau 1985; Lyman 1985)
1.00 (20°C, selected, Suntio et al. 1988)
Henry’s Law Constant (Pa·m3/mol):
- 0.0032 (estimated from Henry’s law constant, Howard 1991)
- 5.6 × 10⁻⁵ (selected, Mackay & Stiver 1991)
- 1.3 × 10⁻⁵, 8.0 × 10⁻⁵, 1.07 × 10⁻³ (quoted, Wauchope et al. 1992)
- 0.00107 (20–25°C, selected, Wauchope et al. 1992)

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 2.81 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
- 2.59 (electrometric titration, Freese et al. 1979)
- 1.57 (Kenaga & Goring 1980, Kenaga 1980b)
- 1.36 (Gerstl & Helling 1987)
- 2.65 (shake flask, Hansch & Leo 1987)
- 2.65 (centrifugal chromatography, Ilchmann et al. 1993)
- 2.81 (recommended, Sangster 1993)
- 2.81 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
- 1.11, −0.097 (calculated-S, $K_{OW}$ Kenaga 1980a)
- 2.46, 1.30 (beef fat, fish, Kenaga 1980b)
- 0.778, 1.94 (alga Chlorella fusca: exp. 24 h exposure, calculated-S, Geyer et al. 1981)
- 0.778, < 1.0, 1.23 (algae, golden orfe, activated sludge, Freitag et al. 1982)
- 0.00 (fish, microcosm conditions, Garten & Trabalka 1983)
- 0.778, 1.23 (algae, calculated-$K_{OW}$ Geyer et al. 1984)
- 1.11 (calculated, Isensee 1991)
- 0.5 (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)

Sorption Partition Coefficient, log $K_{OC}$:
- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
- 1.30, 2.11 (quoted, Kenaga & Goring 1980)
- 1.68, 1.86, 1.68; 1.76 (commerce soil, Tracy soil, Catlin soil; average value of 3 soils, McCall et al. 1981)
- 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)
- 1.61 (soil, quoted, Sabljic 1987)
- 1.75, 2.00 (quoted, calculated-MCI $\chi$, Gerstl & Helling 1987)
- 1.29–2.13 (soil, quoted values, Howard 1991)
- 1.30 (selected, Mackay & Stiver 1991)
- 1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
- 1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted, Wauchope et al. 1992)
- 1.30 (soil, selected, Wauchope et al. 1992)
- 0.68 (calculated-$K_{OW}$, Kollig 1993)

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 soil of 1 cm deep and $t_{1/2} = 7.1$ yr from 10 cm deep (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).
Oxidation: photooxidation $t_{1/2} = 1.8–18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991).

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: degradation kinetics not first-order, time for 50% decomposition in six soils: $t_{1/2} = 5$ d in Commerce soil, $t_{1/2} = 1.5$ d in Catlin soil, $t_{1/2} = 3.9$ d in Keith soil, $t_{1/2} = 3.0$ d in Cecil soil, $t_{1/2} = 2.5$ d in Walla-Walla soil and $t_{1/2} = 8.5$ d in Fargo soil, with an average time of 4 d (McCall et al. 1981); easily degraded under aerobic conditions with $t_{1/2} = 1.8$ and 3.1 d for cometabolism and metabolism respectively, under anaerobic conditions the degradation rate decreases and the $t_{1/2} = 69$ and 135 d (Liu et al. 1981; quoted, Muir 1991);

second-order $k = (3.6–28.8) \times 10^{-6}$ mL·cell$^{-1}$·d$^{-1}$ in natural water (Paris et al. 1981; quoted, Klečka 1985); first-order $k < 0.14–0.07$ d$^{-1}$ in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985); $k = 0.058 \pm 0.006$ d$^{-1}$ in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985; quoted, Muir 1991); $k = 0.08–0.46$ d$^{-1}$ in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$\text{t}_{1/2}^{\text{aq. aerobic}} = 240–1200$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980a, b; quoted, Howard et al. 1991; Muir 1991);

$\text{t}_{1/2}^{\text{aq. anaerobic}} = 672–4320$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991); first-order $k = 0.035$ d$^{-1}$ in die-away test, $k = 0.029$ d$^{-1}$ in CO$_2$ evolution test in soil and $k = 6.9 \times 10^{-1}$ mL·(g bacteria)$^{-1}$·d$^{-1}$ by activated sludge cultures (Scow 1982); biodegradation $t_{1/2} = 18$ to $> 50$ d in clear river water and $t_{1/2} = 10$ to 25 d in muddy water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to $t_{1/2} = 1.8–3.1$ d under aerobic conditions and $t_{1/2} = 69–135$ d under anaerobic conditions (Howard 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8–18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991); photooxidation $t_{1/2} = 23.9$ h for reactions with hydroxyl radicals 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 (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); 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).

Groundwater: $t_{1/2} = 480–4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991).

Soil: $t_{1/2} = 240–1200$ 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); field $t_{1/2} = 2–16$ d, with a selected value of 10 d (Wauchope et al. 1992).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).
### 13.2 SUMMARY TABLES AND QSPR PLOTS

#### TABLE 13.2.1
Summary of physical properties of carboxylic acids

<table>
<thead>
<tr>
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<td><strong>Aliphatics:</strong></td>
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<tr>
<td>Formic acid</td>
<td>64-18-6</td>
<td>HCOOH</td>
<td>46.026</td>
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<td>Acetic acid</td>
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<td>CH&lt;sub&gt;3&lt;/sub&gt;COOH</td>
<td>60.052</td>
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<td>117.9</td>
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<td>Propionic acid</td>
<td>79-09-4</td>
<td>C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;7&lt;/sub&gt;COOH</td>
<td>74.079</td>
<td>–20.5</td>
<td>141.15</td>
<td>1</td>
<td>74.60</td>
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<td>Butyric acid</td>
<td>107-92-6</td>
<td>C&lt;sub&gt;4&lt;/sub&gt;H&lt;sub&gt;9&lt;/sub&gt;COOH</td>
<td>88.106</td>
<td>–5.1</td>
<td>163.75</td>
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<tr>
<td>Isobutyric acid</td>
<td>79-31-2</td>
<td>(CH&lt;sub&gt;3&lt;/sub&gt;)&lt;sub&gt;2&lt;/sub&gt;CHCOOH</td>
<td>88.106</td>
<td>–46</td>
<td>154.45</td>
<td>1</td>
<td>91.00</td>
</tr>
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<td>n-Valeric acid</td>
<td>109-52-4</td>
<td>C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;10&lt;/sub&gt;COOH</td>
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<td>503-74-2</td>
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<td>Trimethylacetic acid</td>
<td>75-98-9</td>
<td>(CH&lt;sub&gt;3&lt;/sub&gt;)&lt;sub&gt;3&lt;/sub&gt;COOH</td>
<td>102.132</td>
<td>35</td>
<td>164</td>
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<td>135.0</td>
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<td>Hexanoic acid (Caproic acid)</td>
<td>142-62-1</td>
<td>C&lt;sub&gt;7&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;COOH</td>
<td>116.158</td>
<td>–3</td>
<td>205.2</td>
<td>1</td>
<td>125.79</td>
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<tr>
<td>Octanoic acid</td>
<td>124-07-2</td>
<td>C&lt;sub&gt;8&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;COOH</td>
<td>144.212</td>
<td>16.5</td>
<td>239</td>
<td>1</td>
<td>201.6</td>
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<td>Stearic acid</td>
<td>57-11-4</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;COOH</td>
<td>248.478</td>
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<td>0.368</td>
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<td>112-80-1</td>
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<td>13.4</td>
<td>360</td>
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<td>79-10-7</td>
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<td>72.063</td>
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<td>2-Butenoic (cis-)</td>
<td>503-64-0</td>
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<td>86.090</td>
<td>15</td>
<td>169</td>
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<td>83.85</td>
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<td>2-Butenoic (trans-)</td>
<td>107-93-7</td>
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<td>Vinylic acid</td>
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<td>162.5</td>
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<tr>
<td>Chloroacetic acid</td>
<td>79-11-8</td>
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<td>189.3</td>
<td>0.424</td>
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<td>Dichloroacetic acid</td>
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<tr>
<td>Benzoic acid</td>
<td>65-85-0</td>
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<td>122.122</td>
<td>122.35</td>
<td>249.2</td>
<td>0.111</td>
<td>134.8</td>
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<td>2-Methylbenzoic acid</td>
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<td>CH&lt;sub&gt;3&lt;/sub&gt;C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt;COOH</td>
<td>136.149</td>
<td>103.5</td>
<td>259</td>
<td>0.170</td>
<td>157.0</td>
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<tr>
<td>3-Methylbenzoic acid</td>
<td>99-04-7</td>
<td>CH&lt;sub&gt;3&lt;/sub&gt;C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;COOH</td>
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<td>109.9</td>
<td>263</td>
<td>0.147</td>
<td>157.0</td>
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<td>4-Methylbenzoic acid</td>
<td>99-94-5</td>
<td>CH&lt;sub&gt;3&lt;/sub&gt;C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;COOH</td>
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<td>76.5</td>
<td>265.5</td>
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<td>88-99-3</td>
<td>C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;1,2-(COOH)&lt;sub&gt;2&lt;/sub&gt;</td>
<td>166.132</td>
<td>230 dec</td>
<td>dec</td>
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<td>118-91-2</td>
<td>CIC&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt;COOH</td>
<td>156.567</td>
<td>140.2</td>
<td>sublim</td>
<td>0.0741</td>
<td>101.4</td>
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<th>Carboxylic Acid</th>
<th>CAS</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>BOiling Point</th>
<th>Sublimation Temperature</th>
<th>ΔHsublim (J/mol)</th>
<th>ΔSsublim (J/mol K)</th>
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<td>158</td>
<td>sublim</td>
<td>0.0496</td>
<td>155.7</td>
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<td>4-Chlorobenzoic acid</td>
<td>74-11-3</td>
<td>ClC₆H₄COOH</td>
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<td>0.00726</td>
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<td>HOC₆H₄COOH</td>
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<td>0.0484</td>
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<td>285 dec</td>
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<td>164.4</td>
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<td>dec</td>
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* Assuming ΔSsublim = 56 J/mol K.
### TABLE 13.2.2
Summary of selected physical-chemical properties of carboxylic acids at 25°C

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<tr>
<th>Compound</th>
<th>Solubility</th>
<th>Selected properties</th>
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<th>Henry's law constant</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H/(Pa·m³/mol)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>calc/C</td>
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<tr>
<td>Aliphatics:</td>
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<tr>
<td>Formic acid</td>
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<td></td>
<td>5750</td>
<td>5750</td>
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<tr>
<td>Acetic acid</td>
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<td>Propionic acid</td>
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<td>435</td>
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<td>Butyric acid</td>
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<td>84</td>
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<td>1.088</td>
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a Brimblecombe et al. 1992; b Hine & Mookerjee 1975.
TABLE 13.2.3
Suggested half-life classes for carboxylic acids in various environmental compartments at 25°C

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<th>Compound</th>
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<td>5</td>
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<td>Butyric acid</td>
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<td>4</td>
<td>5</td>
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<td>5</td>
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<td>Stearic acid (Octadecanoic acid)</td>
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<td>4</td>
<td>5</td>
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<tr>
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<td>4</td>
<td>5</td>
</tr>
<tr>
<td>Vinylacetic acid</td>
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<td>3</td>
<td>4</td>
<td>5</td>
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<td>4</td>
<td>5</td>
<td>6</td>
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<td>3</td>
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<td>5</td>
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where,

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<th>Class</th>
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<th>Range (hours)</th>
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<tr>
<td>2</td>
<td>17 (~1 d)</td>
<td>10–30</td>
</tr>
<tr>
<td>3</td>
<td>55 (~2 d)</td>
<td>30–100</td>
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<td>4</td>
<td>170 (~1 week)</td>
<td>100–300</td>
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<td>5</td>
<td>550 (~3 weeks)</td>
<td>300–1,000</td>
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<td>6</td>
<td>1,700 (~2 months)</td>
<td>1,000–3,000</td>
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<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 y)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>9</td>
<td>~5 y</td>
<td>&gt;30,000</td>
</tr>
</tbody>
</table>
FIGURE 13.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

FIGURE 13.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.
FIGURE 13.2.3 Octanol-water partition coefficient versus Le Bas molar volume for carboxylic acids.

FIGURE 13.2.4 Henry's law constant versus Le Bas molar volume for carboxylic acids.
FIGURE 13.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for carboxylic acids.
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Carboxylic Acids


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  14.1.2.8 2,4,5-Trichlorophenol .................................... 2781
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14.1 LIST OF CHEMICALS AND DATA COMPILATIONS

14.1.1 ALKYLPHENOLS AND OTHER SUBSTITUTED PHENOLS

14.1.1.1 Phenol

Common Name: Phenol

Synonym: carbolic acid, phenic acid, phenylic acid, phenyl hydrate, phenyl hydroxide, hydroxybenzene, oxybenzene

Chemical Name: phenol

CAS Registry No: 108-95-2

Molecular Formula: C₆H₅OH

Molecular Weight: 94.111

Melting Point (°C):
40.89 (Lide 2003)

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

Density (g/cm³ at 20°C):
1.5479 (supercooled liq., Ericksen & Dobbert 1955)
1.0576 (Weast 1982)

Acid Dissociation Constant, pKₐ:
9.90 (Blackman et al. 1955, McLeese et al. 1979)
10.02 (Herington & Kynaston 1957; Callahan et al. 1979)
9.82 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)
10.0 (Serjeant & Dempsey 1979; Paris et al. 1982; Miyake et al. 1987; Tratnyek & Hoigné 1991)
10.05 (Saarikoski 1982; Saarikoski & Viluksela 1982)
9.90 (UV absorption, Hoigné & Bader 1983; Scully & Hoigné 1987)
10.93 (Miyake et al. 1987)
10.12 (UV spectrophotometry, Nendza & Seydel 1988)

Molar Volume (cm³/mol):
89.0 (20°C, calculated-density)
103.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
56.13, 45.83 (25°C, bp, Dreisbach 1955)
47.30 (at normal bp, Biddiscombe & Martin 1958)
45.689 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH[subl] (kJ/mol):
68.66 (at 25°C, Biddiscombe & Martin 1958; Andon et al. 1960)

Enthalpy of Fusion, ΔH_fus (kJ/mol):
11.514 (Riddick et al. 1986)

Entropy of Fusion, ΔS_fus (J/mol K):
36.63 (Tsonopoulos & Prausnitz 1971)
36.0, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.698 (mp at 40.89°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
86600* (synthetic method, measured range 20–65.86°C, Hill & Malisoff 1926)
83000 (20°C, synthetic method, Jones 1929)
89300* (22.7°C, thermostatic and synthetic methods, measured range 22.7–60.9°C, Morrison 1944)
<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Method and Instrument(s)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>shake flask-UV at pH 5.1</td>
<td>Blackman et al. 1955</td>
</tr>
<tr>
<td>20</td>
<td>synthetic method/shake flask-optical</td>
<td>Ericksen &amp; Dobbert 1955</td>
</tr>
<tr>
<td>20</td>
<td>shake flask-spectrophotometry</td>
<td>Roberts et al. 1977</td>
</tr>
<tr>
<td>20</td>
<td>shake flask-GC</td>
<td>Kraij &amp; Sincic 1980</td>
</tr>
<tr>
<td>20</td>
<td>shake flask-UV</td>
<td>Hashimoto et al. 1984</td>
</tr>
<tr>
<td>20</td>
<td>solid-phase microextraction SPME-GC</td>
<td>Buchholz &amp; Pawliszyn 1994</td>
</tr>
<tr>
<td>20</td>
<td>shake flask-conductimetry</td>
<td>Achard et al. 1996</td>
</tr>
<tr>
<td>25.35</td>
<td>shake flask-optical method</td>
<td>Jaoui et al. 1999</td>
</tr>
<tr>
<td>23.15</td>
<td>shake flask-optical method</td>
<td>Jaoui et al. 2002</td>
</tr>
<tr>
<td>ln [S/(\text{mol kg}^{-1})] = 7.3013 – 853.62/(T/K); temp range 288–313 K</td>
<td>Jaoui et al. 2002</td>
<td></td>
</tr>
<tr>
<td>ln [S/(\text{mol kg}^{-1})] = 10.731 – 1931.7/(T/K); temp range 313–332 K</td>
<td>Jaoui et al. 2002</td>
<td></td>
</tr>
</tbody>
</table>

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

133.3* \((44.8 °C, \text{static method-manometer, measured range 44.8–181.4} °C, \text{Kahlbaum 1898})\)

28531* \((141.1 °C, \text{mercury manometer, measured range 141.1–181.1} °C, \text{Goldblum et al. 1947})\)

log \((P/\text{mmHg}) = -2510/(T/K) + 8.395; \text{temp range: 141.1–181.1} °C (\text{Hg manometer, Goldblum et al. 1947})\)

55.54* \((\text{extrapolated-regression of tabulated data, temp range 40.1–181.9} °C, \text{Stull 1947})\)

7605* \((107.15 °C, \text{ebulliometry, measured range 107.15–181.75} °C, \text{Dreisbach & Shrader 1949})\)

1333* \((70.50 °C, \text{ebulliometry, measured range 70.50–181.7 °C, Vonteres et al. 1955})\)

70.75 \((\text{calculated-Antoine eq., Dreisbach 1955})\)

log \((P/\text{mmHg}) = 7.57893 – 1817.0/(205.0 + t/°C), \text{temp range: 93–240} °C, (\text{Antoine eq. for liquid state, Dreisbach 1955})\)

44.26* \((24.85 °C, \text{gas saturation and diaphragm manometer measurements, measured range 0–37.5} °C, \text{Biddiscombe & Martin 1958})\)

45.71 \((\text{gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958})\)

log \((P/\text{mmHg}) = 11.5638 – 3586.36/(t/°C + 273); \text{temp range 9–40} °C (\text{Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960})\)

log \((P/\text{mmHg}) = 7.13457 – 1615.072/(t/°C + 174.569); \text{temp range 110–200} °C (\text{Antoine eq. from reported expptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973})\)

47.00 \((\text{interpolated-Antoine eq., Stephenson & Malanowski 1987})\)

50.2 (selected, Riddick et al. 1986)

45.7, 45.32 \((\text{interpolated-Antoine eq., Stephenson & Malanowski 1987})\)

47.00 \((\text{extrapolated-Antoine eq., Dean 1985})\)

log \((P/\text{mmHg}) = 7.1330 – 1516.79/(174.95 + t/°C); \text{temp range 107–182} °C (\text{Antoine eq. from reported expptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973})\)

26.66, 133.3 \((20 °C, 40 °C, \text{Verschueren 1977, 1983})\)

16.27 \((\text{extrapolated-Cox eq., Chao et al. 1983})\)

log \((P/\text{mmHg}) = -[0.2185 \times 11891.5/(T/K)] + 8.513843; \text{temp range 40.1–418.7} °C (\text{Antoine eq. Weast 1972–73})\)

46.91, 54.74 \((\text{extrapolated-Antoine eq., Boublik et al. 1973})\)

log \((P/kPa) = 6.70346 – 1793.899/(200.218 + t/°C); \text{temp range 70.5–181.7} °C (\text{Antoine eq. from reported expptl. data, Boublik et al. 1984})\)

55.00 \((\text{selected, Riddick et al. 1986})\)

45.7, 45.32 \((\text{interpolated-Antoine eq., Stephenson & Malanowski 1987})\)
log (P/kPa) = 10.6887 – 3586.36/(T/K); temp range 282–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P/kPa) = 10.71099 – 3594.703/(T/K); temp range 273–313 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.25947 – 1516.072/(–98.581 + T/K); temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.34757 – 1482.82/(–113.862 + T/K); temp range 455–655 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.57957 – 1710.287/(–80.273 + T/K); temp range 314–395 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.26694 – 1522.07/(–97.834 + T/K); temp range 387–456 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.30177 – 1548.368/(–94.612 + T/K); temp range 449–526 K (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)
log (PL/kPa) = 6.92874 – 2146.053/(–17.025 + T/K); temp range 520–625 K (Antoine eq.-VIII, liquid, Stephenson & Malanowski 1987)
61.16 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
log (P/Pa) = 37.91650 – 4155.615/(T/K) – 9.02308·log (T/K) + 0.04526 × 10 –2·(T/K); temp range: 394–455 K (four-parameter vapor pressure eq. using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
log (P/Pa) = 127.08645 – 7292.585/(T/K) – 42.92601·log (T/K) + 1.76834 × 10 –2·(T/K); temp interval of inves-
tigation 380–455 K (four-parameter vapor pressure eq. derived using data of Dreisbach & Shrader 1949, Nesterova et al. 1990)
log (P/mmHg) = 23.5332 – 3.4961 × 10 3/(T/K) – 4.899·log (T/K) + 1.216 × 10–4·(T/K) + 9.6537 × 10–13·(T/K)2; temp range 314–694 K (vapor pressure eq., Yaws 1994)
173* (40.09 °C, ebulliometry, measured range 40–90 °C, Tabai et al. 1997)

Henry’s Law Constant (Pa m3/mol at 25 °C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0402 (exp., Hine & Mookerjee 1975; Howard 1989)
0.065, 1.082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.0718* (27.0°C, gas stripping-GC, measured range –2.0 to 27.0°C Abd-El-Bary et al. 1986)
kH/kPa = 2.69 × 108 exp[–6120/(T/K)], temp range –2 to 90°C (gas stripping-GC measurements plus reported data at higher temp., Abd-El-Bary et al. 1986)
1.245, 2.193, 3.322 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
0.0607* (extrapolated from temp dependence eq., Dohnal & Fenclová 1995)
ln KAW = 8.701 – 5760/(T/K), temp range 20–100°C (vapor-liquid equilibrium measurements with additional literature data, Dohnal & Fenclová 1995)
kH/kPa = 670.117 – 39274.5/(T/K) – 94.6679; temp range 313–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)
< 0.240 (gas stripping-GC, Altschuh et al. 1999)
0.0536 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
0.0320* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)
ln [H/(M atm–1)] = 5850/(T/K) – 11.6; temp range 284–302 K, Harrison et al. 2002)
0.157* (dynamic equilibrium/gas stripping-GC/MS, measured range 5–25°C, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, log KOW. Additional data at other temperatures designated * are compiled at the end of this section:
1.46 (shake flask-UV, Fujita et al. 1964)
1.46 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
1.42 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
1.60 (shake flask, Kiezyk & Mackay 1971)
1.47 (Leo et al. 1971)
1.51 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
1.49 (shake flask, Korenman 1972)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value(s)</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.46, 1.61</td>
<td>(LC-k’ correlation, calculated-π const., Carlson et al. 1975)</td>
</tr>
<tr>
<td></td>
<td>1.54</td>
<td>(shake flask-UV, Davis et al. 1976)</td>
</tr>
<tr>
<td></td>
<td>1.45</td>
<td>(HPLC-RT correlation, Mirlees et al. 1976)</td>
</tr>
<tr>
<td></td>
<td>1.48 ± 0.02</td>
<td>(shake flask at pH 7, Unger et al. 1978)</td>
</tr>
<tr>
<td></td>
<td>1.48, 1.46, 1.49, 1.51, 0.62, 2.20 (literature values, Hansch &amp; Leo 1979)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.46</td>
<td>(HPLC-k’ correlation, Butte et al. 1981; Butte et al. 1987)</td>
</tr>
<tr>
<td></td>
<td>1.45</td>
<td>(generator column-HPLC/UV, Wasik et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>1.54</td>
<td>(RP-HPLC-k’ correlation, D’Amboise &amp; Hanai 1982)</td>
</tr>
<tr>
<td></td>
<td>1.28, 1.54 (RP-LC-k’ correlation, calculated-fragment const. as per Rekker 1977, Hanai &amp; Hubert 1982)</td>
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<tr>
<td></td>
<td>1.54</td>
<td>(HPLC-k’ correlation, Miyake &amp; Terada 1982; Miyake et al. 1987)</td>
</tr>
<tr>
<td></td>
<td>1.62</td>
<td>(inter-laboratory, shake flask average, Eadsforth &amp; Moser 1983)</td>
</tr>
<tr>
<td></td>
<td>1.16</td>
<td>(inter-laboratory, HPLC average, Eadsforth &amp; Moser 1983)</td>
</tr>
<tr>
<td></td>
<td>1.49, 1.53 ± 0.09 (selected best lit. value, exptl.-ALPM, Garst 1984)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.46, 1.55 ± 0.07 (selected best lit. value, exptl.-ALPM, Garst &amp; Wilson 1984)</td>
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<tr>
<td></td>
<td>1.08</td>
<td>(calculated-activity coeff. γ from UNIFAC, Campbell &amp; Luthy 1985)</td>
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<tr>
<td></td>
<td>1.46</td>
<td>(RP-HPLC-RT correlation, Chin et al. 1986)</td>
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<tr>
<td></td>
<td>1.00, 1.42 (HPLC-k’ correlation, Eadsforth 1986)</td>
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<tr>
<td></td>
<td>1.46</td>
<td>(shake flask-CPC centrifugal partition chromatography, Berthod et al. 1988)</td>
</tr>
<tr>
<td></td>
<td>1.46</td>
<td>(RP-HPLC-capacity ratio correlation, Mínick et al. 1988)</td>
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<tr>
<td></td>
<td>1.46</td>
<td>(HPLC-RT correlation, Shigeota et al. 1988)</td>
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<tr>
<td></td>
<td>1.52 ± 0.01 (filter chamber-UV, Hersey et al. 1989)</td>
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<td></td>
<td>1.50</td>
<td>(recommended, Sangster 1989, 1993)</td>
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<tr>
<td></td>
<td>1.52, 1.58, 1.69 (CPC-RV correlation, Gluck &amp; Martin 1990)</td>
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<tr>
<td></td>
<td>1.47</td>
<td>(shake flask-UV, Kramer &amp; Henze 1990)</td>
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<tr>
<td></td>
<td>1.37 ± 0.06 (liquid-liquid extraction-flow injection-UV, Kubá 1991)</td>
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</tr>
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<td></td>
<td>1.57</td>
<td>(shake flask-GC, Kishino &amp; Kobayashi 1994)</td>
</tr>
<tr>
<td></td>
<td>1.46</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
</tbody>
</table>

**Bioconcentration Factor, log BCF:**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value(s)</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.16</td>
<td>(total 14C in fathead minnow, mean exposure level 0.0025 µg·mg⁻¹, Call et al. 1980)</td>
</tr>
<tr>
<td></td>
<td>4.23</td>
<td>(total 14C in fathead minnow, mean exposure level 0.0327 µg·mg⁻¹, Call et al. 1980)</td>
</tr>
<tr>
<td></td>
<td>4.20</td>
<td>(total 14C in fathead minnow, mean value, Call et al. 1980)</td>
</tr>
<tr>
<td></td>
<td>2.20</td>
<td>(goldfish, rate constant ratio k₁/k₂, Nagel &amp; Urich 1980)</td>
</tr>
<tr>
<td></td>
<td>0.97</td>
<td>(microorganisms-water, calculated-K_{OC}, Mabey et al. 1982)</td>
</tr>
<tr>
<td></td>
<td>1.30, 2.30, 3.34 (golden ide, algae, activated sludge, Freitag et al. 1985)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.30</td>
<td>(chlorella fusca, Freitag et al. 1985; quoted, Howard 1989)</td>
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<tr>
<td></td>
<td>1.20</td>
<td>(algae, maximum apparent BCF, Hardy et al. 1985)</td>
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<tr>
<td></td>
<td>0.544</td>
<td>(algae, real BCF with biotransformation, Hardy et al. 1985)</td>
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<tr>
<td></td>
<td>3.14</td>
<td>(daphnia magna, estimated-¹³C activity and on dry wt. basis, Dauble et al. 1986)</td>
</tr>
<tr>
<td></td>
<td>2.44</td>
<td>(daphnia magna, based on elimination phase, Dauble et al. 1986)</td>
</tr>
<tr>
<td></td>
<td>1.28</td>
<td>(daphnia magna, Dauble et al. 1986; quoted, Geyer et al. 1991)</td>
</tr>
<tr>
<td></td>
<td>1.24</td>
<td>(zebrafish, Butte et al. 1987)</td>
</tr>
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</table>

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

<table>
<thead>
<tr>
<th>Property</th>
<th>Value(s)</th>
<th>Source(s)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>1.43</td>
<td>(soil, Kenaga &amp; Goring 1980)</td>
</tr>
<tr>
<td></td>
<td>1.48</td>
<td>(20°C, sorption isotherm, converted form K_{OM} organic carbon in soils, Briggs 1981)</td>
</tr>
<tr>
<td></td>
<td>1.15</td>
<td>(sediment-water, calculated-K_{OC}, Mabey et al. 1982)</td>
</tr>
<tr>
<td></td>
<td>1.57, 1.96</td>
<td>(silt loams, Scott et al. 1983, quoted, Howard 1989)</td>
</tr>
<tr>
<td></td>
<td>3.46</td>
<td>(untreated fine sediment, Isaacson &amp; Frink 1984)</td>
</tr>
<tr>
<td></td>
<td>3.49</td>
<td>(untreated coarse sediment, Isaacson &amp; Frink 1984)</td>
</tr>
<tr>
<td></td>
<td>1.35</td>
<td>(HPLC-k’ correlation, mobile phase buffered to pH 3, Hodson &amp; Williams 1988)</td>
</tr>
<tr>
<td></td>
<td>2.17</td>
<td>(soil, calculated-K_{OC}, Howard 1989)</td>
</tr>
<tr>
<td></td>
<td>2.4, 2.43</td>
<td>(soil: quoted, calculated-MCI χ, Meylan et al. 1992)</td>
</tr>
</tbody>
</table>
2.68, 2.38 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100, 200 mmol/kg at pH 7, shake flask-sorption isotherm, Li et al. 2000)
1.43 (soil, calculated-MCI χ, Sabljic et al. 1995)
1.42, 1.00, 1.24 (RP-HPLC-k correlation on 3 different stationary phases, Szabo et al. 1995)
1.59, 1.67 (HP/LC-k correlation, C18 column, Hong et al. 1996)
1.32, 2.43 (HPLC-screening method; calculated-PCOC fragment method, Müller & Kördel 1998)
1.56, 1.556, 1.307, 1.52 (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)
1.31, 1.75, 1.26, 1.67 (RP:LC-k′ correlation, C18 column, Hong et al. 1996)
1.56, 1.556, 1.255, 1.307, 1.52 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
1.31, 1.75, 1.26, 1.67 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
1.37, 1.34 (soils: organic carbon OC ≥ 0.1% and pH 3.2–7.4, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-lives, t½:
Volatilization: estimated t½ ~ 3.2 months for evaporation from water (Howard 1989);

\[ t_{\text{½}} = 88 \text{ d} \]

Photolysis: phototransformation rate \( k = 0.015 \text{ h}^{-1} \) with \( t_{\text{½}} = 46 \text{ h} \) in the summer (mean temp 24°C) and \( k = 0.0040 \text{ h}^{-1} \) with \( t_{\text{½}} = 173 \text{ h} \) in the winter (mean temp 10°C) in distilled water; \( k = 0.018 \text{ h}^{-1} \) with \( t_{\text{½}} = 39 \text{ h} \) in the summer and \( k = 0.0074 \text{ h}^{-1} \) with \( t_{\text{½}} = 94 \text{ h} \) in the winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);

\[ \text{photomineralization rate } k = 0.04 \text{ h}^{-1} \text{ with } t_{\text{½}} = 16 \text{ d} \text{ in the summer and } k = 0.0041 \text{ h}^{-1} \text{ with } t_{\text{½}} = 169 \text{ d} \text{ in the winter in distilled water; } k = 0.0055 \text{ h}^{-1} \text{ with } t_{\text{½}} = 7 \text{ d} \text{ in the summer and } k = 0.0010 \text{ h}^{-1} \text{ with } t_{\text{½}} = 73 \text{ d} \text{ in the winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);} \]

atmospheric \( t_{\text{½}} = 46 \text{ to } 173 \text{ h}, \text{ based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter; aquatic photolysis } t_{\text{½}} = 46 \text{ to } 173 \text{ h}, \text{ based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter (Howard et al. 1991)} \]

Apparent first-order rate constant phototransformation at \( \lambda > 285 \text{ nm} \), \( k = (3.10 \pm 0.10) \times 10^{-2} \text{ h}^{-1} \) in purified water (Zamy et al. 2004)

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

\[ k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with RO2 radical at } 30^\circ \text{C in aquatic systems with } t_{\text{½}} > 100 \text{ yr (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)} \]

\[ k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with singlet oxygen at } 25^\circ \text{C with } t_{\text{½}} > 100 \text{ yr (Foote 1976; Mill 1979; quoted, Mill 1982)} \]

\[ k_{\text{NO3}} = (2.0 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } (300 \pm 1) \text{ K (Carter et al. 1981)} \]

\[ k = 6.5 \times 10^8 \text{ s}^{-1} \text{, dye-sensitized photooxidation first-order rate constant, second order } k = (1.3 \pm 0.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in water using } 1 \text{ mM PrOH as scavenger at pH 1.7–2.0 and 20–23^\circ C (Hoigné & Bader 1983a)} \]

\[ k_{\text{NO3}} = (2.10 \pm 0.50) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (Atkinson et al. 1984)} \]

\[ k_{\text{NO3}} = (3.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294 \text{ K with reference to reaction for NO3 radical with 2-methyl-2-butene (Atkinson et al. 1984; quoted, Atkinson 1991)} \]

\[ k_{\text{OH}(\text{exptl})} = 28.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{OH}(\text{calc})} = 45.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1985)} \]

\[ k_{\text{OH}(\text{calc})} = 36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ and } k_{\text{OH}(\text{obs})} = 28.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)} \]

\[ k = (2 \text{ to } 3) \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH } 8, 1.9 \times 10^7 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH } 9, 4.6 \times 10^6 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH 9.5, 9.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1} at pH 10 and 1.8 \times 10^7 \text{ M}^{-1} \text{ s}^{-1} at pH 11.5 for the reaction with singlet oxygen at (19 \pm 2)^\circ C in water (Scully & Hoigné 1987)} \]

\[ k_{\text{NO3}} = 3.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)} \]

\[ k_{\text{OH}} = 26.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1990)} \]

\[ k_{\text{NO3}} = (2.59 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \pm 1 \text{ K with reference to reaction for NO3 radicals with cis-2-butene (Atkinson 1991)} \]
k = (2.6 ± 4) × 10^6 M⁻¹ s⁻¹ for the reaction with singlet oxygen in aqueous phosphate buffer at (27 ± 1)°C (Tratyniek & Hoigné 1991)

k_{OH} = 10.45 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, k_{NO₃} = 11.44 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (Müller & Klein 1991)

k_{NO₃} = (3.92 ± 0.25) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K with reference to reaction for NO₃ radical with 2-methyl-2-butene; k_{OH} = 26.5 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson et al. 1992)

k_{OH(calc)} = 12 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital estimation method, Klamt 1993)

k_{OH} = (2.6 ± 0.25) × 10⁻¹² cm³ molecule⁻¹ s⁻¹, and k_{OH(aq.)} = 6.7 × 10⁻¹⁰ M⁻¹ s⁻¹, the calculated atmospheric lifetime τ = 0.45 d under clear sky; τ = 0.38 d under cloudy conditions at 298 K, reduced to 0.26 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

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

Biodegradation: t½ = 1–2 d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

decomposition by soil microflora within 1 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)

complete disappearance in soil suspensions in 2 d (Woodcock 1971; quoted, Verschueren 1983)

k_B = 80.0 mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20–d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

k_B = (0.094 ± 0.003) h⁻¹ at feed concentration of 180 mg/L at 20°C and k = (0.095 ± 0.007) h⁻¹ at feed concentration of 360 mg/L at 20°C in a continuous stirred reactor (Beltrame et al. 1984)

k_B = 0.035 d⁻¹ with t_σ = 20 d in ground water; k_B = 0.065 d⁻¹ with t_σ = 11 d in Lester River water;

k_B = 0.247 d⁻¹ with t_σ = 3 d in Superior harbor waters (Vaishnav & Babeu 1987)

k_B = 0.03 h⁻¹ and t_σ = 28 h for estuarine water in summer (mean temp 24°C) and k_B = 0.011 h⁻¹ with t_σ = 62 h in winter (mean temp. 10°C); k_B = 0.4 h⁻¹ with t_σ = 2 d in summer and k_B = 0.0051 h⁻¹ with t_σ = 146 d in winter in darkness with microbes (Hwang et al. 1986)

k_B = 0.041–0.028 h⁻¹ in 10–100 mg/L sludge (Urano & Kato 1986)

complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with t_σ = 9 d in estuary river (Howard 1989)

k_B(exptl., average) = 0.0498 h⁻¹; k_B(calc) = 0.0545 h⁻¹ (nonlinear) and k_B(calc) = 0.0503 h⁻¹ (linear) (group contribution method, Tabak & Govind 1993)

t_σ(aerobic) = 0.25 d, t_σ(anaerobic) = 8.0 d in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation k = (7.1 ± 1.3) × 10⁻¹² L·organism⁻¹ h⁻¹ (Paris et al. 1982); estimated bacterial transformation k = 3 × 10⁻⁶ mL·cell⁻¹ h⁻¹ in water (Mabey et al. 1982); microbial transformation rate constants in pond and river samples k = (2.0 ± 1.5) × 10⁻¹⁰ to (4.8 ± 3.1) × 10⁻¹⁰ L·organism⁻¹ h⁻¹ at five different sites (Paris et al. 1983; quoted, Steen 1991); degradation rate constants k = 1.08 × 10⁻¹⁶ mol·cell⁻¹ h⁻¹ from pure culture studies and k = 0.90 × 10⁻¹² to 3.00 × 10⁻¹² mol·cell⁻¹ h⁻¹ with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

k₁ = 3.15 h⁻¹; k₂ = 0.02 h⁻¹ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: t_σ = 0.61 d by reaction with OH radicals in air (Howard 1989);

k = 0.0462 d⁻¹ corresponding to t_σ = 360 h in air (Guine & Heijungs 1993);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994); calculated lifetimes of 5.3 h and 9.0 min for reactions with OH, NO₃ radical, respectively (Atkinson 2000), atmospheric lifetime τ = 0.45 d under clear sky and τ = 0.38 d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to τ = 0.26 d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: rate constant k = (1.3 ± 0.2) × 10⁻¹⁰ M⁻¹ s⁻¹ for the reaction with ozone at pH 2.0–6.0 (Hoigné & Bader 1983);

k_B = 46 h in summer, t_σ = 173 h in winter in distilled water and t_σ = 39 h in summer, t_σ = 94 h in winter in estuarine water, based on phototransformation rate when exposed to full sunlight and microbes (Hwang et al. 1986)

k_B = 43 h in summer, t_σ = 118 h in winter in poisoned estuarine water, based on photo-transformation rate and t_σ = 384 h or 16 d in summer, t_σ = 2640 h or 110 d in winter in poisoned estuarine water, based on photomineralization rate (Hwang et al. 1986);
Phenolic Compounds

\( t_{1/2} = 384 \text{ h or 16 d in summer, } t_{1/2} = 4056 \text{ h or 169 d in winter in distilled water; and } t_{1/2} = 168 \text{ h or 7 d in summer, } t_{1/2} = 1752 \text{ h or 73 d in winter in estuarine water, based on photo-mineralization rate when exposed to full sunlight and microbes (Hwang et al. 1986); } \)

\( t_{1/2} = 2000 \text{ h in water at pH 8 and } 19 \pm 2^\circ\text{C for the reaction with singlet oxygen (Scully & Hoigné 1987); } \)

\( t_{1/2} = 11 \text{ d in river waters and } t_{1/2} = 3 \text{ d in Superior harbor waters (Vaishnav & Babeu 1987); } \)

\( t_{1/2} = 77 \text{ to 3840 h in water, based on reported reaction rate constant for RO}_2\text{ radical with the phenols class, } t_{1/2} = 5.3 \text{ to 56.5 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991); } \)

\( \text{degradation rate constant } k = 0.0217 \text{ d}^{-1} \text{ corresponding to a } t_{1/2} = 766 \text{ h in water (quoted from Howard 1989, Guinee & Heijungs 1993)} \)

\( t_{1/2}(\text{aerobic}) = 0.25 \text{ d, } t_{1/2}(\text{anaerobic}) = 8 \text{ d in natural waters (Capel & Larson 1995)} \)

Groundwater: biodegradation \( t_{1/2} = 20 \text{ d (Vashinav & Babeu 1987); } \)

\( t_{1/2} = 12 \text{ to 168 h, based on estimated aerobic biodegradation half-life (Howard et al. 1991). } \)

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 2 d in Dunkirk silt loam, 1 d in Mardin silt loam (Alexander & Aleem 1961)

degradation in soil completed in 2–5 d even in subsurface soils and \( t_{1/2} = 2.70 \text{ and 3.51 h of low concentration of phenol in 2 silt loam soils (Howard 1989); } \)

\( t_{1/2} = 24 \text{ to 240 h, based on aerobic soil die-away data (Howard et al. 1991); } \)

\( t_{1/2} = 4.1 \text{ d in a slightly basic sandy loam soil containing 3.25% organic matter and } t_{1/2} = 23 \text{ d in acidic clay soil with } <1\% \text{ organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992)} \)

\( \text{degradation rate constant } k = 0.227 \text{ d}^{-1} \text{ corresponding to a } t_{1/2} = 73.3 \text{ h in soil (quoted from Howard 1989, Guinee & Heijungs 1993). } \)

Biota: elimination from goldfish within 4 h (Nagel & Urich 1980);

\( \text{depuration } t_{1/2}(\text{obs}) = 336 \text{ h, } t_{1/2}(\text{calc}) = 385 \text{ h for exposure level of 0.0025 } \mu\text{g mL}^{-1} \text{ and } t_{1/2}(\text{obs}) = 438 \text{ h, } t_{1/2}(\text{calc}) = 497 \text{ h for exposure level of 0.0375 } \mu\text{g mL}^{-1} \text{ (Call et al. 1980); } \)

\( \text{depuration } t_{1/2}(\text{calc}) = 8 \text{ to 44 min in algae (Hardy et al. 1985); } \)

\( \text{half-lives in fish } t_{1/2} < 1 \text{ d for goldfish, } t_{1/2} = 14–18 \text{ d for minnow (Niimi 1987)} \)

---

**TABLE 14.1.1.1.1**

**Reported aqueous solubilities of phenol at various temperatures**

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### TABLE 14.1.1.1.1 (Continued)

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Some data from Achard et al. 1996, Jaoui et al. 1999

**FIGURE 14.1.1.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for phenol.
### TABLE 14.1.1.2
Reported vapor pressures of phenol at various temperatures and the coefficients for the vapor pressure equations

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

1. **Kahlbaum 1898**

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*complete list see ref.

2. **Vonterres et al. 1955**

<table>
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<th>t/°C</th>
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<th>t/°C</th>
<th>P/Pa</th>
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*complete list see ref.

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**TABLE 14.1.1.2 (Continued)**

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<th>t/°C</th>
<th>P/Pa</th>
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Antoine eq. for temp range: 0–40°C

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<th>eq. 2</th>
<th>P/mmHg</th>
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<td>A</td>
<td>11.5638</td>
<td>A</td>
<td>7.13457</td>
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<tr>
<td>B</td>
<td>3586.36</td>
<td>B</td>
<td>1516.072</td>
</tr>
<tr>
<td>C</td>
<td>273</td>
<td>C</td>
<td>174.569</td>
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</table>

**FIGURE 14.1.1.2** Logarithm of vapor pressure versus reciprocal temperature for phenol.
TABLE 14.1.1.3
Reported Henry's law constants of phenol at various temperatures and temperature dependence equations

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

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>gas stripping-GC/FID</strong></td>
<td><strong>vapor-liquid equilibrium</strong></td>
<td><strong>derived from measured P</strong></td>
<td><strong>gas stripping-GC/MS</strong></td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
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<td>-2.0</td>
<td>0.0072</td>
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<td>100.0</td>
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<td>0.0607#</td>
<td>20.0</td>
<td>0.0605$</td>
</tr>
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<td>eq. 3</td>
<td>k_P/kPa</td>
<td>eq. 1</td>
<td><strong>K_{AW}</strong></td>
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<tr>
<td>A</td>
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<td>eq. 1</td>
<td><strong>K_{AW}</strong></td>
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<tr>
<td>B</td>
<td>6120.0</td>
<td>A</td>
<td>8.701</td>
</tr>
<tr>
<td>$A \quad \text{derived included lit. data}$</td>
<td>$B \quad \text{derived included lit. data}$</td>
<td>$A \quad \text{derived included lit. data}$</td>
<td>$B \quad \text{derived included lit. data}$</td>
</tr>
</tbody>
</table>

Enthalpy of hydration:

\[
\Delta H_k/(\text{kJ mol}^{-1}) = 47.9 \pm 0.5 \quad \text{OR}
\]

\[
\Delta H_k/(\text{kJ mol}^{-1}) = 50.2 \pm 0.4 \quad \text{eq. 4}
\]

<table>
<thead>
<tr>
<th><strong>gas stripping-GC/MS</strong></th>
<th><strong>H/(M atm⁻¹)</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m³/mol)</strong></td>
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<tr>
<td>284</td>
<td>0.0122</td>
</tr>
<tr>
<td>284.5</td>
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<td>289.5</td>
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<td>293.5</td>
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<tr>
<td>298</td>
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<td>302</td>
<td>0.0379</td>
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<tr>
<td>298.5</td>
<td>0.0199</td>
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<tr>
<td>eq. 4</td>
<td>H/(M atm⁻¹)</td>
</tr>
<tr>
<td>B</td>
<td>-5850</td>
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</tbody>
</table>
FIGURE 14.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for phenol.

TABLE 14.1.1.4
Reported octanol-water partition coefficients of phenol at various temperatures

Korenman & Udalova 1974

<table>
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<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
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<tbody>
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<td>1.531</td>
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<tr>
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<tr>
<td>50</td>
<td>1.396</td>
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<tr>
<td>60</td>
<td>1.369</td>
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</table>

\[ \log K_{OW} = A - B/(T/K) \]

A 0.4479

B -305.877
FIGURE 14.1.1.4 Logarithm of $K_{OW}$ versus reciprocal temperature for phenol.
### 14.1.1.2 o-Cresol

![Structure of o-Cresol](image)

**Common Name:** o-Cresol  
**Synonym:** 2-hydroxytoluene, 2-methylphenol, o-cresylic acid, o-hydroxytoluene, 2-cresol, 1,2-cresol  
**Chemical Name:** 2-methylphenol  
**CAS Registry No:** 95-48-7  
**Molecular Formula:** C₇H₈O, C₆H₄(CH₃)OH  
**Molecular Weight:** 108.138

<table>
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<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>31.03 (Lide 2003)</td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>191.04 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm² at 20°C)</td>
<td>1.0273 (Weast 1982–83)</td>
</tr>
<tr>
<td>Acid Dissociation Constant, pKₐ</td>
<td>10.28 (Pearce &amp; Simkins 1968)</td>
</tr>
<tr>
<td></td>
<td>10.20 (Hoigné &amp; Bader 1983; Weast 1982–83)</td>
</tr>
<tr>
<td></td>
<td>10.26 (Dean 1985)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>104.4 (30°C, Stephenson &amp; Malanowski 1987)</td>
</tr>
<tr>
<td></td>
<td>125.6 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, ΔHᵥ (kJ/mol)</td>
<td>46.94 (Biddiscombe &amp; Martin 1958)</td>
</tr>
<tr>
<td></td>
<td>45.91 (at normal boiling point, Andon et al. 1960)</td>
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<td></td>
<td>42.7 (Dean 1992)</td>
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<tr>
<td>Enthalpy of Sublimation, ΔHₛₘₜₜ (kJ/mol)</td>
<td>76.02 (at 25°C, Biddiscombe &amp; Martin 1958; Andon et al. 1960; Dean 1992)</td>
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<td>Enthalpy of Fusion, ΔHₖₚᵤₜ (kJ/mol)</td>
<td>15.8 (Tsonopoulos &amp; Prausnitz 1971; Riddick et al. 1986)</td>
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<td>Entropy of Fusion ΔSₖₚᵤₜ (J/mol K)</td>
<td>52.01 (Tsonopoulos &amp; Prausnitz 1971)</td>
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<tr>
<td>Fugacity Ratio at 25°C (assuming ΔSₖₚᵤₜ = 56 J/mol K), F:</td>
<td>0.873 (mp at 31.03°C)</td>
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</tbody>
</table>

**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):  
30100* (35.3°C, shake flask, measured range 35.3–162.8°C, critical solution temp 162.8°C, Sidgwick et al. 1915)  
24970 (shake flask-residue volume method, Booth & Everson 1948)  
25950 (shake flask-UV at pH 5.1, Blackman et al. 1955)  
25000* (20°C, synthetic method/shake flask-optical, measured range 0–166.5°C, Ericksen & Dobbert 1955)  
25000 (shake flask-UV spectrophotometry, Roberts et al. 1977)  
2725 (generator column-HPLC, Wasik et al. 1981)  
31000, 56000 (40°C, 100°C, Verschueren 1983)  
42608, 48061, 52241 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)  
26800 (shake flask-HPLC/UV at pH 3.6, Varhaníčková 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):  
23065* (142.3°C, mercury manometer, measured range 142.3–190.8°C, Goldblum et al. 1947)
Phenolic Compounds

log (P/mmHg) = \( -2520/(T/\text{K}) + 8.308 \); temp range 142.3–177.1 °C (Hg manometer, Goldblum et al. 1947)

58.16* (extrapolated-regression of tabulated data, temp range 38–190.5 °C, Stull 1947)

7605* (113.11 °C, ebulliometry, measured range 113.11–190.95 °C, Dreisbach & Shrader 1949)

56.72 (calculated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = \( 7.49476 – 1777.8/(T/\text{K}) \); temp range 97–250 °C (Antoine eq. for liquid state, Dreisbach 1955)

38.60 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)

37.32* (25.25 °C, gas saturation -diaphragm manometer, temp range 0–28 °C, Biddiscombe & Martin 1958)

log (P/mmHg) = \( 7.07055 – 3970.17/(T/\text{K} + 273) \); temp range 110–200 °C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin 1958; Andon et al. 1960)

30.7 (extrapolated-Antoine eq., Boublík et al. 1973)

log (P/mmHg) = \( 6.91172 – 1435.5/(-96.04 + T/\text{K}) \); temp range 120–191 °C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublík et al. 1984)

32.0 (Verschueren 1977, 1983)

38.32 (extrapolated-Cox eq., Chao et al. 1983)

log (P/mmHg) = \( [1– 463.986/(T/\text{K})] \times 10^{1.01555 – 9.95980 \times 10^{-4 \cdot (T/\text{K}) + 7.92834 \times 10^{-7 \cdot (T/\text{K})^2}} \); temp range 313.20–697.65 K (Cox eq., Chao et al. 1983)

30.3, 22.5 (extrapolated-Antoine eq., Boublík et al. 1984)

log (P/kPa) = \( 6.02377 – 1427.165/(164.218 + T/\text{K}) \); temp range 120–191 °C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublík et al. 1984)

log (P/kPa) = \( 5.82809 – 1299.971/(148.886 + T/\text{K}) \); temp range 142.3–189.8 °C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

30.74 (extrapolated-Antoine eq., Dean 1985)

log (P/kPa) = \( 6.9117 – 1435.5/(165.16 + T/\text{K}) \); temp range 120–191 °C (Antoine eq., Dean 1985, 1992)

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

log (P/kPa) = \( 11.68858 – 3909.409/(T/\text{K}) \); temp range 273–303 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P/kPa) = \( 6.19545 – 1542.299/(-96.04 + T/\text{K}) \); temp range 383–473 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log (P/kPa) = \( 6.47616 – 1714.489/(-79.841 + T/\text{K}) \); temp range 304–409 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

log (P/kPa) = \( 6.19561 – 1543.097/(-95.902 + T/\text{K}) \); temp range 399–470 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

log (P/kPa) = \( 6.24893 – 1584.403/(-90.794 + T/\text{K}) \); temp range 463–526 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)

log (P/kPa) = \( 6.82237 – 2134.352/(-19.536 + T/\text{K}) \); temp range 517–630 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)

40.0 (Riddick et al. 1986)

39.4 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)

log (P/Pa) = \( 99.85294 – 6347.665/(T/\text{K}) – 32.60231 \cdot \log (T/\text{K}) + 1.24267 \times 10^{-2 \cdot (T/\text{K})^2} \); temp interval of investigation: 412–467 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)

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

0.124, 0.07, 1.082 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.284, 0.162 (8, 25 °C, calculated, Leuenberger et al. 1985)

0.0852 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

0.176* (°C, calculated-activity coeff. γ∞ data, measured range 25–35 °C, Dohnal & Fenclová 1995)
3.352, 5.386, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
0.178 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
ln \( K_{\text{AW}} \) = 9.091 – 5556/(T/K), temp range 20–100 °C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
0.159 (gas stripping-GC, Altschuh et al. 1999)
0.102 (calculated-group contribution, Lee et al. 2000)
0.217 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
0.0965* (gas stripping-UV, measured range 281–302 K, Harrison et al. 2002)
ln [H/(M atm –1)] = 6680/(T/K) – 15.4; temp range 281–302 K, Harrison et al. 2002)
0.146, 0.239* (20, 25 °C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):  
2.04 (shake flask-UV, Korenman & Pereshein 1970)
1.95 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
1.95 (LC-K’ correlation, Carlson et al. 1975)
2.045 (shake flask, Korenman et al. 1980)
2.17 (HPLC-K’ correlation, Butte et al. 1981; Butte et al. 1987)
1.96 (generator column-HPLC, Wasik et al. 1981)
1.99 (RP-HPLC-K’ correlation, Miyake & Terada 1982)
1.98 (recommended, Sangster 1989)
1.97, 1.98 (COMPUTOX data bank, Kaiser 1993)
1.95 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:  
1.26 (calculated-K\( _{\text{OW}} \), Lyman et al. 1982; quoted, Howard 1989)
1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):  
1.34 (Brookstone clay loam soil at pH 5.7, Boyd 1982; quoted, Howard 1989)
1.26 (calculated-S, Boyd 1982; quoted, Howard 1989)
1.76 (calculated-K\( _{\text{OW}} \), Kollig 1993)

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

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( K_{\text{OH}} \) for reaction with OH radical, \( K_{\text{NO}_3} \) with NO3 radical and \( K_{\text{O}_3} \) with O3 or as indicated, *data at other temperatures see reference:
\( k_{\text{OH}} = 3.41 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 300 ± 1 K (relative rate method with reference to 2-methyl-2-butene Perry et al. 1977; Atkinson et al. 1979)
\( k_{\text{NO}_3} = (12 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 300 ± 1 K (relative rate method with reference to with 2-methyl-2-butenes Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)
\( k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1} \) for oxidation with singlet oxygen at 25°C in the aquatic system with half-life > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
\( k_{\text{OH}} = 20 \times 10^8 \text{ M}^{-1} \text{ s}^{-1} \) at 25°C with \( t_\text{1/2} = 0.3 \text{ d} \) (Hendry & Kenley 1979; quoted, Mill 1982)
\( k_{\text{NO}_3} = (13.9 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 300 ± 1 K (relative rate method with reference to the reaction of NO3 radical with 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)
photooxidation \( t_\text{1/2} = 66–3480 \text{ h} \) in water, based on reaction rate constants for OH and \( \text{RO}_2 \) radicals with the phenol class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)
\( k_{\text{O}_3} = (2.55 \pm 0.39) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 ± 2 K; calculated tropospheric lifetimes of 45 d and 0.3 d due to reaction with O3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)
\( k_{\text{OH}} = 2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \) with half-life of 0.3 d in the atmosphere (Mill 1982)
\( k_{\text{OH}} = 2.0 \times 10^3 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \) at 300 K (Lyman et al. 1982)
\( k = (1.2 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1} \) for the reaction with ozone in water at pH 1.5–2.0 (Hoigne & Bader 1983b)
Phenolic Compounds

\[ k_{OH} = 4.1 \times 10^{-11} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}, k_{NO_3} = 1 \times 10^{-11} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K} \text{ (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)}

\[ k_{NO_3} = (1.20 \pm 0.34) \times 10^{-11} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K} \text{ (Atkinson et al. 1984)}

\[ k_{NO_3} = (15.6 \pm 1.7) \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ with reference to the reaction of NO}_3 \text{ radical with m-cresol at } (298 \pm 1) \text{ K} \text{ (Atkinson et al. 1984; quoted, Atkinson 1991)}

\[ k_{OH} = 40 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ for the vapor-phase reaction with } 5 \times 10^3 \text{ hydroxyl radical/cm}^3 \text{ at room temp. and a loss rate of } 1.7 \text{ d}^{-1} \text{ (Atkinson 1985; quoted, Howard et al. 1991)}

\[ k_{OH}(\text{exptl}) = 37 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1}, \text{ and } k_{OH}(\text{calc}) = 44.8 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1985)}

\[ k_{OH}(\text{exptl}) = 40 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 44 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)}

\[ k_{OH} = 4.2 \times 10^{-11} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (recommended, Atkinson 1989, 1990)}

\[ k_{NO_3} = (13.7 \pm 0.9) \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ at } (296 \pm 2) \text{ K, and } k_{OH} = 42 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ for at room temp. (Atkinson et al. 1992)}

\[ k_{OH}(\text{calc}) = 30.36 \times 10^{-12} \text{ cm}^3\text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}

\[ k_{OH} = 4.9 \times 10^{-11} \text{ cm}^3\text{ mol}^{-1} \text{ s}^{-1}, \text{ and } k_{OH}(\text{aq.}) = 1.1 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1}, \text{ the calculated atmospheric lifetime } \tau = 0.24 \text{ d under clear sky; } \tau = 0.22 \text{ d under cloudy conditions at } 298 \text{ K, reduced to 0.17 d due the average temperature of tropospheric clouds at } 283 \text{ K (Feigenbrugel et al. 2004)}

Hydrolysis:

Biodegradation: 1 to 2 d for bacteria to utilize 95% of 300 ppm in the parent substrate (Tabak et al. 1964)

\[ t_{1/2} = 2 \text{ d at } 20^\circ\text{C and 7 d at } 4^\circ\text{C in river water (Ludzack & Ettinger 1960; quoted, Howard 1989)}

completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschuren 1983);

average rate of biodegradation \( k = 54.0 \text{ mg COD g}^{-1} \text{ h}^{-1} \text{ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)}\)

\[ t_{1/2}(\text{aq. aerobic}) = 24–168 \text{ h, based on unacclimated aerobic screening test data (Takemoto et al. 1981; Urushigawa et al. 1983; quoted, selected, Howard et al. 1991)}\]

\[ t_{1/2}(\text{aq. anaerobic}) = 96–672 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)}\]

\[ k(\text{exptl.}) = 0.0679 \text{ h}^{-1} \text{ compared to group contribution method predicted } k(\text{calc}) = 0.0728 \text{ h}^{-1} \text{ (nonlinear) and } k = 0.0567 \text{ h}^{-1} \text{ (linear) (Tabak & Govind 1993)}\]

\[ t_{1/2}(\text{aerobic}) = 2 \text{ d, } t_{1/2}(\text{anaerobic}) = 15 \text{ d in natural waters (Capel & Larson 1995)}\]

Biotransformation: microbial transformation \( k = (2.7 \pm 1.3) \times 10^{-10} \text{ L‧organism}^{-1}\text{‧h}^{-1} \text{ (Paris et al. 1983; quoted, Steen 1991)}\)

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

Half-Lives in the Environment:

Air: photooxidation \( t_{1/2} = 1.6–16 \text{ h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)}\)

loss rate \( k = 10.8 \times 10^{-4} \text{ min}^{-1} \text{ in outdoor Teflon chambers in the dark (Grosjean 1985)}\)

photodegradation \( t_{1/2} = 9.6 \text{ h in air, based on measured rate constant for the reaction with photochemically generated hydroxyl radicals (quoted, Howard 1989)}\)

atmospheric transformation lifetime \( \tau < 1 \text{ d (estimated, Kelly 1994)}\)

calculated lifetimes of 2.2 h, 2 min and 65 d for reactions with OH radical, NO\(_3\) radical and O\(_3\), respectively (Atkinson 2000).

calculated atmospheric lifetime \( \tau = 0.24 \text{ d under clear sky and } \tau = 0.22 \text{ d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at } 298 \text{ K, reduced to } \tau = 0.19 \text{ d due to average temperature of tropospheric cloud at } 283 \text{ K (Feigenbrugel et al. 2004)}\)

Surface water: photooxidation \( t_{1/2} = 66–3480 \text{ h in water, based on reaction rate constants for OH and RO\(_2\) radicals with the phenol class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)}\)

rate constant \( k = (1.2 \pm 0.3) \times 10^{4} \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983)}\)

\[ t_{1/2}(\text{aerobic}) = 2 \text{ d, } t_{1/2}(\text{anaerobic}) = 15 \text{ d in natural waters (Capel & Larson 1995)}\]

Ground water: estimated \( t_{1/2} \sim 0.01 \text{ yr for cresols at Noordwijk (Zoeteman et al. 1981)}\).
Sediment:
Soil: $t_{1/2} = 24$–$168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} = 5.1$ d in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 1.6$ d in slightly basic sandy loam soil with $3.25\%$ organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

**TABLE 14.1.1.2.1**

Reported aqueous solubilities of $o$-cresol at various temperatures

<table>
<thead>
<tr>
<th>Sidgwick et al. 1915</th>
<th>Erichsen &amp; Dobbert 1955</th>
<th>Dohnal &amp; Fenclová 1995</th>
</tr>
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<td>shake flask-synthetic method</td>
<td>shake flask-optical method</td>
<td>vapor-liquid equil.-UV</td>
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<td>$t$/°C</td>
<td>$S$/g·m$^{-3}$</td>
<td>$t$/°C</td>
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<tr>
<td>-------------------------------------</td>
<td>-------------------------------</td>
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<td>29.9</td>
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Critical solution temp 162.8° C
Triple point 8° C
**FIGURE 14.1.1.2.1** Logarithm of mole fraction solubility \((\ln x)\) versus reciprocal temperature for \(-\text{o-cresol.}\)

**TABLE 14.1.1.2.2**

Reported vapor pressures of \(-\text{o-cresol at various temperatures and the coefficients for the vapor pressure equations}\)

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

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<tr>
<th>(T/°C)</th>
<th>(P/Pa)</th>
<th>(m.p/°C)</th>
<th>(\text{mp}^\circ\text{C})</th>
<th>eq. 1</th>
<th>(P/mmHg)</th>
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<tr>
<td>38.2</td>
<td>133.3</td>
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### TABLE 14.1.1.2.2 (Continued)

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<td>ebulliometry</td>
<td>gas saturation</td>
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<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
<td>$t/°C$</td>
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<tr>
<td>$\text{bp/°C}$</td>
<td>191.003</td>
<td>191.046</td>
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<td>for temp range:</td>
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<td>$0–30^°C$</td>
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<tr>
<td>eq. 2</td>
<td>$P/\text{mmHg}$</td>
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<tr>
<td>$A$</td>
<td>11.5638</td>
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<td></td>
</tr>
<tr>
<td>$B$</td>
<td>3586.36</td>
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</tr>
<tr>
<td>$C$</td>
<td>273</td>
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<tr>
<td>$\Delta H_v/(\text{kJ mol}^{-1})$</td>
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<tr>
<td>at $\text{bp}$</td>
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<td>at $25^°C$</td>
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**FIGURE 14.1.1.2.2** Logarithm of vapor pressure versus reciprocal temperature for $o$-cresol.

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TABLE 14.1.1.2.3
Reported Henry's law constants of o-cresol at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \\
\ln (1/K_{AW}) &= A - B/(T/K) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \\
\ln H &= A - B/(T/K) + C(T/K)^2 \\
K_{AW} &= A - B·(T/K) + C·(T/K)^2 \\
\end{align*}
\]

\(1\) \hspace{1cm} (1) \hspace{1cm} \log K_{AW} = A - B/(T/K) \hspace{1cm} (1a) \\
\(2\) \hspace{1cm} (2) \hspace{1cm} \log (1/K_{AW}) = A - B/(T/K) \hspace{1cm} (2a) \\
\(3\) \hspace{1cm} (3) \hspace{1cm} \log k_H = A - B/(T/K) \hspace{1cm} (3a) \\
\(4\) \hspace{1cm} (4) \hspace{1cm} \log H = A - B/(T/K) \hspace{1cm} (4a) \\
\(5\) \hspace{1cm} (5) \\

Dohnal & Fenclová 1995 \hspace{1cm} Harrison et al. 2002 \hspace{1cm} Feigenbrugel et al. 2004

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>T/K</th>
<th>H/(Pa m³/mol)</th>
<th>T/K</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
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<td>25</td>
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<tr>
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<td>B -6680</td>
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</tr>
</tbody>
</table>

#calculated from eq. 1
$calculated from eq. 3
*data from literature

eq. 1 \hspace{1cm} K_{AW} 
A \hspace{1cm} 9.091
B \hspace{1cm} 5556

enthalpy of hydration:
\(\Delta H_k/(kJ \ mol^{-1}) = 46.2 \pm 0.4 \)

OR

eq. 3 \hspace{1cm} k_H/kPa
A \hspace{1cm} 21.832
B \hspace{5827}
\(\Delta H_k/(kJ \ mol^{-1}) = 48.5 \pm 0.4 \)

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**FIGURE 14.1.1.2.3** Logarithm of Henry's law constant versus reciprocal temperature for o-cresol.
14.1.1.3  

**m-Cresol**

Common Name: *m*-Cresol

Synonym: *m*-cresylic acid, 1-hydroxy-3-methylbenzene, 3-hydroxytoluene, *m*-hydroxytoluene, 3-methylphenol, *m*-methylphenol, 3-cresol

Chemical Name: *m*-cresol, 3-methylphenol

CAS Registry No: 108-39-4

Molecular Formula: C\(_7\)H\(_8\)O, C\(_6\)H\(_4\)(CH\(_3\))OH

Molecular Weight: 108.138

Melting Point (°C):
12.24  (Lide 2003)

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

Density (g/cm\(^3\)):
1.0336  (Weast 1982–83)
1.0302  (25°C, Riddick et al. 1986)

Acid Dissociation Constant, pK\(_a\):
10.09  (Pearce & Simkins 1968; Riddick et al. 1986; Howard 1989)
10.0  (Hoigné & Bader 1983; Dean 1985)
10.01  (Weast 1982–83)

Molar Volume (cm\(^3\)/mol):
105.6  (calculated-density, Rohrschneider 1973)
125.6  (calculated-Le Bas-method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
49.38  (at normal bp, Biddiscombe & Martin 1958)
47.40  (at normal boiling point, Andon et al. 1960)
61.714  (at 25°C, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Sublimation, \(\Delta H_{sub}\) (kJ/mol):
6.53  (Tsonopoulos & Prausnitz 1971)
10.70  (Riddick et al. 1986; Dean 1992)

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

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. Additional data at other temperatures designated * are compiled at the end of this section):
23600*  (24.7°C, shake flask, measured range –2 to 87.58°C, critical solution temp 147°C, Sidgwick et al. 1915)
22664  (shake flask-residue volume method, Booth & Everson 1948)
22000*  (20°C, synthetic method/shake flask-optical, measured range 0–148°C, Ericksen & Dobbert 1955)
25000  (shake flask-spectrophotometry, Roberts et al. 1977)
2800  (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
23500, 58000  (20°C, 100°C, Verschueren 1977, 1983)
23790*  (20.35°C, equilibrium cell-concn ratio-GC, measured range 20.35–139°C, Leet et al. 1987)
46935, 54615, 58327(75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
19600  (shake flask-HPLC/UV at pH 4.45, Varhaníčková 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 the section):

- **20265** (149.5°C, mercury manometer, measured range 149.5–201.1°C, Goldblum et al. 1947)
  \[ \log (P/\text{mmHg}) = -2650/(T/\text{K}) + 8.457; \text{ temp range 149.5–201.1°C (Hg manometer, Goldblum et al. 1947)} \]

- **23.95** (extrapolated-regression of tabulated data, temp range 52–202.8°C, Stull 1947)

- **25.83** (calculated-Antoine eq., Dreisbach 1955)
  \[ \log (P/\text{mmHg}) = 7.53165 – 1875.3/(201.0 + t/°C), \text{ temp range: 110–240°C, (Antoine eq. for liquid state, Dreisbach 1955)} \]

- **1333** (85.5°C, ebulliometry, measured range 85.5–202.1°C, Vonterres et al. 1955)

- **18.278** (24.90°C, gas saturation-diaphragm manometer, temp range 0–39°C, Biddiscombe & Martin 1958)
  \[ \log (P/\text{mmHg}) = 9.9653 – 3223.45/(t/°C + 273); \text{ temp range 11–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)} \]


- **36.43** (calculated-Cox eq., Chao et al. 1983)
  \[ \log (P/\text{mmHg}) = [–0.2185 × 13483.8/(T/\text{K})] + 9.135933; \text{ temp range 52–202.8°C (Antoine eq., Weast 1972–73)} \]

- **22.1, 11.9** (extrapolated-Antoine eq., Dean 1985)

- **79960** (466.35 K, vapor-liquid equilibrium, measured range 466.35–588.68 K, Klara et al. 1987)

- **19.08; 18.61** (interpolated-Antoine eq.-III, IV, Stephenson & Malanowski 1987)

- **2.628394 – 1603.811/(–100.232 + T/K); temp range 410–477 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)**


- **19.0** (extrapolated-Antoine eq., Nesterova et al. 1990)

- **log (P/\text{Pa}) = 5272.296/(T/K) – 18.84252 \times 10^{-2}/(T/K); temp range: 409–477 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)**

- **log (P/mmHg) = 105.528 – 6.9748 × 10^{3}/(T/K) – 35.083 \times 10^{-2}/(T/K) – 2.4317 \times 10^{-12}/(T/K)^{2}; \text{ temp range 285–706 K (vapor pressure eq., Yaws 1994)}**
Henry’s Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0203, 0.0881 (8, 25°C, calculated, Leuenberger et al. 1985)
0.0875, 0.0627 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)
0.0718 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
0.01068 (calculated-P/C, Shiu et al. 1994)
0.0810, 0.0865* (24.7, 25°C, calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
1.683, 2.990, 4.635 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
0.0848 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)

ln K_{AW} = 8.909 – 5722/(T/K), temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

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

1.96 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1985)
2.02 (shake flask, Korenman et al. 1980)
1.94 (HPLC-RT correlation, Butte et al. 1981)
1.96 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
1.96 (shake flask-UV, Saarikoski & Viluksela 1982)
1.98 (recommended, Sangster 1989, 1993)
1.96 (COMPUTOX databank, Kaiser 1993)
1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.30 (golden ide, after 3 d, Freitag et al. 1985)
3.69 (algae, after 1 d, Freitag et al. 1985)
3.04 (activated sludge, after 5 d, Freitag et al. 1985)
1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log K_{OC}:

1.54 (Brookstone clay loam soil, Boyd 1982)
1.26 (calculated-S, Boyd 1982)
1.76 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, and Half-Lives, t_½:

Volatilization:

Photolysis: direct aqueous photolysis k = 0.011 ± 0.001 min⁻¹ with t_½ = 60.4 min (Stegeman et al. 1993).

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_{NO3} = (7 ± 1) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with reference to the reaction of NO₃ radical with 2-methyl-2-butene (Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

k_{OH} = 48 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with reference to the reaction of OH radical with 2-methyl-2-butene (Atkinson et al. 1979; Carter et al. 1981)

k_{O3} = (8.10 ± 1.16) × 10⁻¹⁵ cm³ molecule⁻¹ s⁻¹ at (300 ± 1) K with reference to the reaction of NO₃ radical with 2-methyl-2-butene (Carter et al. 1981; quoted, Atkinson 1991)

k_{O3} = (1.94 ± 0.35) × 10⁻¹⁰ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K; calculated tropospheric lifetimes of 60 d and 0.2 d due to reaction with O₃ and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

photooxidation half-life of 66–3480 h in water, based on reported reaction rate constants for OH and RO₂ radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

k = (1.3 ± 0.3) × 10⁴ M⁻¹ s⁻¹ for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

k_{OH} = 5.92 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)
**k_{NO3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K} \text{ (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)}**

**k_{NO3} = (9.20 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K} \text{ (Atkinson et al. 1984)}**

**k_{NO3} = (15.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \pm 1 \text{ K with reference to the reaction of NO}_3 \text{ radical with phenol} \text{ (Atkinson et al. 1984; quoted, Atkinson 1991)}**

**k_{OH}^{\text{(calc)}} = 93.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } k_{OH}^{\text{(exptl)}} = 57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \text{ (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)}**

**k_{OH} = 6.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (recommended, Atkinson 1989, 1990)}**

**k_{NO3} = (9.74 \pm 0.74) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with reference to the reaction of NO}_3 \text{ radical with 2-methyl-2-butene, and } k_{OH} = 64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \text{ (Atkinson et al. 1992)}**

**k_{OH}^{\text{(calc)}} = 34.42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}**

**k_{OH} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \text{ the calculated atmospheric lifetime } \tau = 0.22 \text{ d under clear sky; } \tau = 0.19 \text{ d under cloudy conditions at } 298 \text{ K, reduced to } 0.13 \text{ d due the average temperature of tropospheric clouds at } 283 \text{ K (Feigenbrugel et al. 2004)}**

**Hydrolysis:**

**Biodegradation:**

**Hydrolysis: t_{1/2} = 1–2 d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964) completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschueren 1983)**

**average rate k = 55.0 mg COD g^{-1}h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)**

**t_{1/2}(aq. aerobic) = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991)**

**t_{1/2}(aq. anaerobic) = 360–1176 h, based on anaerobic screening test data (Horowitz et al. 1982; Shelton & Tiedje 1981; selected, Howard et al. 1991).**

**Biotransformation:**

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

**Half-Lives in the Environment:**

**Air:**

**t_{1/2} = 8.0 h, based on rate constant for the gas phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);**

**photooxidation t_{1/2} = 1.1–11.3 h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);**

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

**calculated atmospheric lifetime \tau = 0.22 d under clear sky and \tau = 0.19 d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to \tau = 0.13 d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)**

**Surface water:**

**t_{1/2} = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);**

**k = (1.3 \pm 0.3) \times 10^{4} \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983);**

**photooxidation t_{1/2} = 66–3480 h in water, based on reported reaction rate constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991).**

**Ground water:**

**estimated half-life for cresols, t_{1/2} = 0.01 yr at Noordwijk (Zoeteman et al. 1981);**

**t_{1/2} = 96–1176 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).**

**Sediment:**

**Soil:**

**t_{1/2} = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);**

**t_{1/2} = 11.3 d in an acidic clay soil with < 1.0% organic matter and t_{1/2} = 0.6 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).**

**Biota:**
### TABLE 14.1.1.3.1
Reported aqueous solubilities of \( m \)-cresol at various temperatures

<table>
<thead>
<tr>
<th>Method</th>
<th>Temperature (°C)</th>
<th>Solubility (S/g·m⁻³)</th>
<th>Method</th>
<th>Temperature (°C)</th>
<th>Solubility (S/g·m⁻³)</th>
<th>Method</th>
<th>Temperature (°C)</th>
<th>Solubility (S/g·m⁻³)</th>
<th>Method</th>
<th>Temperature (°C)</th>
<th>Solubility (S/g·m⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sidgwick et al. 1915</td>
<td>shake flask-synthetic</td>
<td>-0.20</td>
<td>22400</td>
<td>24.7</td>
<td>23600</td>
<td>47.0</td>
<td>26600</td>
<td>61.9</td>
<td>30300</td>
<td>74.5</td>
<td>35400</td>
</tr>
<tr>
<td>Erichsen &amp; Dobbert 1955</td>
<td>shake flask-optical</td>
<td>0</td>
<td>20000</td>
<td>20</td>
<td>22000</td>
<td>40</td>
<td>25000</td>
<td>60</td>
<td>31000</td>
<td>80</td>
<td>40000</td>
</tr>
<tr>
<td>Leet et al. 1987</td>
<td>equilibrium cell-conc</td>
<td>20.35</td>
<td>23790</td>
<td>24.7</td>
<td>23600</td>
<td>25</td>
<td>22000</td>
<td>40.05</td>
<td>25390</td>
<td>58.45</td>
<td>30190</td>
</tr>
<tr>
<td>Dohnal &amp; Fenclová 1995</td>
<td>vapor-liquid equil.-UV</td>
<td>24.7</td>
<td>24125</td>
<td>25</td>
<td>23194</td>
<td>75.8</td>
<td>46935</td>
<td>88.7</td>
<td>54615</td>
<td>98.5</td>
<td>58327</td>
</tr>
</tbody>
</table>

Critical solution temp: 147°C

mp/°C 4.0

**FIGURE 14.1.1.3.1** Logarithm of mole fraction solubility (ln \( x \)) versus reciprocal temperature for \( m \)-cresol.
### TABLE 14.1.1.3.2
Reported vapor pressures of m-cresol at various temperatures and the coefficients for the vapor pressure equations

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

1. Stull 1947

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (mmHg)</th>
<th>log P (KPa)</th>
<th>ln P (KPa)</th>
<th>Vapor Pressure (KPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>52.0</td>
<td>133.3</td>
<td>149.5</td>
<td>20265</td>
<td>85.5</td>
</tr>
<tr>
<td>76.0</td>
<td>666.6</td>
<td>164.3</td>
<td>33464</td>
<td>105.2</td>
</tr>
<tr>
<td>87.8</td>
<td>1333</td>
<td>179.6</td>
<td>53862</td>
<td>121.7</td>
</tr>
<tr>
<td>101.4</td>
<td>2666</td>
<td>187.4</td>
<td>67328</td>
<td>131.6</td>
</tr>
<tr>
<td>116.0</td>
<td>5333</td>
<td>192.1</td>
<td>76927</td>
<td>139.1</td>
</tr>
<tr>
<td>125.8</td>
<td>7999</td>
<td>196.3</td>
<td>86526</td>
<td>150.0</td>
</tr>
<tr>
<td>138.0</td>
<td>13332</td>
<td>201.1</td>
<td>98925</td>
<td>158.5</td>
</tr>
<tr>
<td>157.3</td>
<td>26664</td>
<td>149.6</td>
<td>20398</td>
<td>163.1</td>
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<td>179.0</td>
<td>53329</td>
<td>154.1</td>
<td>23731</td>
<td>170.1</td>
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<td>202.8</td>
<td>101325</td>
<td>176.4</td>
<td>48796</td>
<td>173.0</td>
</tr>
<tr>
<td>mp°C</td>
<td>10.8</td>
<td>183.4</td>
<td>60128</td>
<td>178.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>201.1</td>
<td>98925</td>
<td>183.5</td>
</tr>
</tbody>
</table>

2. Biddiscombe & Martin 1958

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (mmHg)</th>
<th>log P (KPa)</th>
<th>ln P (KPa)</th>
<th>Vapor Pressure (KPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.00*</td>
<td>135.835</td>
<td>12174</td>
<td>114.99</td>
</tr>
<tr>
<td>4.90</td>
<td>2.933*</td>
<td>149.804</td>
<td>20418</td>
<td>121.25</td>
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<tr>
<td>7.20</td>
<td>4.533*</td>
<td>157.610</td>
<td>26762</td>
<td>127.46</td>
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<tr>
<td>9.15</td>
<td>4.40*</td>
<td>163.741</td>
<td>32816</td>
<td>133.4</td>
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<tr>
<td>11.0</td>
<td>5.866</td>
<td>169.814</td>
<td>39930</td>
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<td>15.0</td>
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<td>174.784</td>
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<td>156.29</td>
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<td>17.65</td>
<td>9.866</td>
<td>179.331</td>
<td>53388</td>
<td>167.90</td>
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<tr>
<td>19.80</td>
<td>11.47</td>
<td>182.979</td>
<td>59446</td>
<td>187.33</td>
</tr>
<tr>
<td>21.50</td>
<td>14.13</td>
<td>186.818</td>
<td>66415</td>
<td>203.4</td>
</tr>
<tr>
<td>24.90</td>
<td>18.27</td>
<td>190.266</td>
<td>73225</td>
<td>216.72</td>
</tr>
<tr>
<td>26.95</td>
<td>27.73</td>
<td>193.424</td>
<td>79951</td>
<td>eq. 3 P/kPa</td>
</tr>
<tr>
<td>29.75</td>
<td>30.80</td>
<td>196.418</td>
<td>86769</td>
<td>A 15.5337</td>
</tr>
<tr>
<td>30.85</td>
<td>36.80</td>
<td>199.003</td>
<td>93024</td>
<td>B 4594.0</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>C 54.34</td>
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### TABLE 14.1.1.3.2 (Continued)

<table>
<thead>
<tr>
<th></th>
<th>Biddiscombe &amp; Martin 1958</th>
<th>Nasir et al. 1980</th>
<th>Klara et al. 1987</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>gas saturation</td>
<td>ebulliometry</td>
<td>diaphragm gauge</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>33.25</td>
<td>43.20</td>
<td>199.694</td>
<td>94754</td>
</tr>
<tr>
<td>39.10</td>
<td>57.60</td>
<td>200.250</td>
<td>96156</td>
</tr>
<tr>
<td>*solid</td>
<td></td>
<td>200.658</td>
<td>97201</td>
</tr>
<tr>
<td></td>
<td></td>
<td>201.216</td>
<td>98639</td>
</tr>
<tr>
<td>bp/°C</td>
<td>202.231</td>
<td>201.557</td>
<td>99550</td>
</tr>
<tr>
<td></td>
<td></td>
<td>202.156</td>
<td>101118</td>
</tr>
<tr>
<td>Antoine eq. for temp range: 11–40°C</td>
<td></td>
<td>202.737</td>
<td>102665</td>
</tr>
<tr>
<td>eq. 2</td>
<td>P/mmHg</td>
<td>Antoine eq. for temp range 110–200°C</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>9.9653</td>
<td>A</td>
<td>7.15904</td>
</tr>
<tr>
<td>B</td>
<td>3223.45</td>
<td>B</td>
<td>1603.811</td>
</tr>
<tr>
<td>C</td>
<td>273</td>
<td>C</td>
<td>172.646</td>
</tr>
<tr>
<td>∆H_v/(kJ mol⁻¹)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>at bp</td>
<td>49.375</td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>61.714</td>
<td></td>
<td></td>
</tr>
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</table>

**FIGURE 14.1.1.3.2** Logarithm of vapor pressure versus reciprocal temperature for *m*-cresol.
### TABLE 14.1.1.3.3
Reported Henry's law constants of \textit{m}-cresol at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>T/°C</th>
<th>H/(Pa m³/mol)</th>
<th>T/K</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.7</td>
<td>0.0810*</td>
<td>278.15</td>
<td>0.0148</td>
</tr>
<tr>
<td>25.0</td>
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# calculated from eq. 1
$ calculated from eq. 3
* data from literature

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enthalpy of hydration: \( \Delta H_f/(kJ mol^{-1}) = 47.6 \pm 0.5 \)

OR

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\( \Delta H_f/(kJ mol^{-1}) = 49.8 \pm 0.6 \)
**FIGURE 14.1.3.3** Logarithm of Henry's law constant versus reciprocal temperature for *m*-cresol.
14.1.1.4  \( p \)-Cresol

\[
\text{OH}
\]

Common Name: \( p \)-Cresol
Synonym: \( p \)-cresylic acid, 1-hydroxy-4-methylbenzene, 4-hydroxytoluene, 4-methylphenol, \( p \)-hydroxytoluene, \( p \)-methylphenol, 4-cresol
Chemical Name: 4-methylphenol
CAS Registry No: 106-44-5
Molecular Formula: \( \text{C}_7\text{H}_8\text{O} \), \( \text{CH}_3\text{C}_6\text{H}_4\text{OH} \)
Molecular Weight: 108.138
Melting Point (°C):
34.77  (Lide 2003)
Boiling Point (°C):
201.98  (Lide 2003)
Density (g/cm\(^3\) at 20°C):
1.0178  (Weast 1982–83)

Acid Dissociation Constant, \( \text{pK}_a \):
10.28  (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)
10.17  (Weast 1982–83)

Molar Volume (cm\(^3\)/mol):
125.6  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
49.53  (at normal bp, Biddiscombe & Martin 1958)
47.55  (at normal boiling point, Andon et al. 1960)
43.2  (Dean 1992)

Enthalpy of Sublimation, \( \Delta H_{\text{subl}} \) (kJ/mol):
73.93  (at 25°C, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
12.72  (Tsonopoulos & Prausnitz 1971; Dean 1992)

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

Enthalpy Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F: 0.802 (mp at 34.77°C)

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):
22400*  (40.2°C, shake flask, measured range 40.2–143.5°C, critical solution temp 143.5°C, Sidgwaick et al. 1915)
24230  (shake flask-residue volume method, Booth & Everson 1948)
19000  (shake -flask-UV, Blackman et al. 1955)
17000*  (20°C, synthetic method/shake flask-optical, measured range 0–143.7°C, Ericksen & Dobbert 1955)
21000  (shake flask-spectrophotometry, Roberts et al. 1977)
24000, 53000 (40°C, 100°C, Verschueren 1977, 1983)
21500*  (calculated-activity coeff. \( \gamma \) data, Dohnal & Fenclová 1995)
43534, 50064, 54615  (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
22000  (shake flask-HPLC/UV at pH 3.9, Varhaníčkova 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):
17599*  (145.7 °C, mercury manometer, measured range 145.7–200.8 °C, Goldblum et al. 1947)
log (P/mmHg) = –2680/(T/K) + 8.524; temp range 145.7–200.9°C (Hg manometer, Goldblum et al. 1947)
21.89* (extrapolated-regression of tabulated data, temp range 53–201.8°C, Stull 1947)
7605* (128.65 °C, ebulliometry, measured range 128.65–201.88 °C, Dreisbach & Shrader 1949)
26.34 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.52971 – 1872.4/(201.0 + t/°C); temp range 97–250°C (Antoine eq. for liquid state, Dreisbach 1955)
15.91 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
12.93* (23.35°C, gas saturation-diaphragm manometer, measured range 0–34.15°C, Biddiscombe & Martin 1958)
log (P/mmHg) = 7.11767 – 1566.029/(t/°C + 167.68); temp range 110–200°C (Antoine eq. from gas-saturation-diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
26.34 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 122.8998 – 7.6175 × 10⁻³(T/K) – 41.637·log (T/K) + 1.5709 × 10⁻²·(T/K)²; temp range 308–705 K (vapor pressure eq., Yaws 1994)
16.1 (extrapolated-Antoine eq., Nesterova et al. 1990)
log (P/Pa) = 93.42570 – 6409.054/(T/K) – 29.82622·log (T/K) + 1.03314 × 10⁻²·(T/K)²; temp range 308–705 K (vapor pressure eq., Yaws 1994)
15.6 (calculated-Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0802; 0.0699; 1.0820 (exptl., calculated-group contribution; calculated-bond contribution Hine & Mookerjee 1975)
0.0223, 0.0973 (8, 25°C, calculated, Leuenberger et al. 1985)
0.689 (calculated-P/C, Neely & Blau 1985)
0.0397 (calculated-VLE vapor liquid equilibrium data, Yaws et al. 1991)
0.0653 (calculated-P/C, Shiu et al. 1994)
0.0783*, 0.297 (25, 40.2°C, calculated-activity coeff. $\gamma^\infty$ data, Dohnal & Fenclová 1995)
1.735, 3.144, 4.774 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
0.0801 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)

$\ln K_{\text{AW}} = 9.328 – 5865/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

< 0.347 (gas stripping-GC, Altschuh et al. 1999)
0.102 (calculated-group contribution, Lee et al. 2000)
0.0582, 0.0989* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
1.94 (shake flask-UV, Fujita et al. 1964)
1.92, 1.94, 1.95 (quoted literature values, Leo et al. 1971; Hansch & Leo 1979, Hansch & Leo 1985)
1.99 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
1.94 (LC-$k'$ correlation, Carlson et al. 1975)
2.17 (shake flask, Korenman et al. 1980)
1.97 (RP-HPLC-$k'$ correlation, Miyake & Terada 1982)
1.92, 1.98 ± 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
1.62 (HPLC-$k'$ correlation, Haky & Young 1984)
1.73 (calculated-activity coeff. $\gamma$ from UNIFAC, Campbell & Luthy 1985)
1.91 (HPLC-$k'$ correlation, Miyake et al. 1987)
1.94 (RP-HPLC-capacity ratio, Minick et al. 1988)
1.94 (recommended, Hansch et al. 1995)
1.90; 2.06, 2.12, 1.94 (solid-phase microextraction; calculated-$K_{\text{OW}}$ program, calculated-CLOGP, quoted exptl., Dean et al. 1996)
1.53, 1.53, 1.69, 1.76 (HPLC-$k'$ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

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

Bioconcentration Factor, log BCF:
1.26 (estimated-$K_{\text{OW}}$, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log $K_{\text{OC}}$:
2.81 (Coyote Creek sediment, Smith et al. 1978)
1.69 (Brookstone clayloam soil, Boyd 1982)
–0.046 (predicted-S, Boyd 1982)
1.76 (calculated-$K_{\text{OW}}$, Kollig 1993)
2.70 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
2.15, 2.33 (soils: organic carbon OC ≥ 0.1% and pH 2.0–7.4, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_1/2$:
Volatilization: $t_1/2$ ~167 d, estimated from a lake as calculated from equations of Mackay & Wolkoff 1973 (Smith et al. 1978).
Photolysis:
$k = 6.8 \times 10^{-7} \text{ s}^{-1}$ under overcast weather of April at 25°C; $t_1/2$ ~ 4800 h in river, $t_1/2$ > 10000 h in both eutrophic lake and pond and $t_1/2$ = 2400 h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978; quoted, Howard 1989) photolytic $t_1/2$ = 5800 h in aquatics (Haque et al. 1980).
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
photooxidation \( t_\text{ox} = 144-11325 \) h in water, based on measured rate data for reactions with singlet oxygen and hydroxyl radical in aqueous solution (Anbar & Neta 1967; Scully & Hoigne 1987; quoted, Howard et al. 1991)

\[ k_{\text{NO}_3} = (13 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \pm 1 \text{ K} \] (Japar & Niki 1975; Graham & Johnston 1978; quoted, Carter et al. 1981)

\[ k_{\text{OH}} = 58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \pm 1 \text{ K} \] (Atkinson et al. 1979; quoted, Carter et al. 1981)

photooxidation \( t_\text{ox} = 10 \) h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson et al. 1979; quoted, Howard 1989)

\[ k_{\text{NO}_3} = (15 \pm 2.4) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \pm 1 \text{ K} \] (relative rate technique with reference to 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

\[ k_{\text{O}_3} = (4.71 \pm 0.66) \times 10^{-19} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K} \] (Atkinson et al. 1982, 1984; Atkinson 1985)

\[ k = (3.0 \pm 0.6) \times 10^4 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with singlet oxygen in water at pH 1.5/2.0} \] (Scully & Hoigne 1987)

\[ k_{\text{OH}} = 21.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \] (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

\[ k_{\text{OH}} = 4.7 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \] (recommended, Atkinson 1989, 1990)

\[ k = (9.6 \pm 2.8) \times 10^6 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with singlet oxygen in aqueous phosphate buffer at } (27 \pm 1)^{\circ} \text{C} \] (Tratnyek & Hoigne 1991)

\[ k_{\text{NO}_3} = (10.7 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K}, k_{\text{OH}} = 47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \] (Atkinson et al. 1992)

\[ k_{\text{OH}} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \text{ and } k_{\text{OH(aq.)}} = 1.2 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1} \] (molecular orbital calculations, Klamt 1993)

\[ k_{\text{OH}} = 1.7 \text{ d}^{-1} \text{ in river water}, k = 0.8-4.7 \text{ d}^{-1} \text{ in estuary water and } k = 2.8-4.8 \text{ d}^{-1} \text{ in marine water after a lag period} \] (Vashon & Schwab 1982; quoted, Battersby 1990)

\[ t_\text{uw(aq. aerobic)} = 1-16 \text{ h}, \text{ based on unacclimated marine and freshwater grab sample data} \] (Van Veld & Spain 1983; Rogers et al. 1984; selected, Howard et al. 1991)
t_{1/2}(a q. anaerobic) = 240–672 h, based on anaerobic screening test data (Boyd et al. 1983; Horowitz et al. 1982; selected, Howard et al. 1991);
k = 1.72 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1} \text{ in pure culture system (Banerjee et al. 1984).}

Biotransformation: estimated $t_{1/2} = 12 \text{ h in river, eutrophic lake and pond and } t_{1/2} > 10000 \text{ h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978).}$

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 10 \text{ h, based on measured rate data for the vapor phase reaction with OH radical in air}$ (Atkinson et al. 1979; quoted, Howard 1989);
photooxidation $t_{1/2} = 1.5–15 \text{ h, based on measured rate data for the vapor phase reaction with OH radical in air}$ (Atkinson 1985; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
calculated atmospheric lifetime $\tau = 0.23 \text{ d under clear sky and } \tau = 0.18 \text{ d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at } 298 \text{ K, reduced to } \tau = 0.11 \text{ d due to average temperature of tropospheric cloud at } 283 \text{ K (Feigenbrugel et al. 2004).}$

Surface water: $t_{1/2} = 0.55 \text{ h in river, } t_{1/2} = 12 \text{ h in pond and eutrophic lake, and } t_{1/2} = 2400 \text{ h in oligotrophic lake}$ for a point source continuously discharging 1.0 \( \mu \text{g/mL predicted by one compartment model for all processes including dilution (Smith et al. 1978; quoted, Howard 1989);}$
rate constant $k = (3.0 \pm 0.6) \times 10^3 \text{ M}^{-1} \text{.s}^{-1}$ for the reaction with ozone at pH 1.5/2.0 in water (Hoigné & Bader 1983b);
$t_{1/2} = 1–16 \text{ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);}$
$t_{1/2} = 500 \text{ h for the reaction with singlet oxygen in water at pH 8 and } (19 \pm 2)°C (Scully & Hoigné 1987).$

Ground water: estimated half-life for cresols, $t_{1/2} = 0.01 \text{ yr at Noordwijk (Zoeteman et al. 1981); } t_{1/2} = 2–672 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).}$

Sediment:

Soil:
$t_{1/2} = 1–16 \text{ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);}$
$t_{1/2} = 0.5 \text{ d in an acidic clay soil with < 1.0% organic matter and } t_{1/2} = 1.0 \text{ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).}$

Biota:
### TABLE 14.1.1.4.1
Reported aqueous solubilities of $p$-cresol at various temperatures

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<th>Sidgwick et al. 1915</th>
<th>Erichsen &amp; Dobbert 1955</th>
<th>Dohnal &amp; Fenclová 1995</th>
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Critical solution temp 143.5°C
Triple point 8.7°C
**FIGURE 14.1.1.4.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for $p$-cresol.

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**TABLE 14.1.1.4.2**

Reported vapor pressures of $p$-cresol at various temperatures and the coefficients for the vapor pressure equations

- $\log P = A - B/(T/K)$ (1)
- $\ln P = A - B/(T/K)$ (1a)
- $\log P = A - B/(C + t/°C)$ (2)
- $\ln P = A - B/(C + t/°C)$ (2a)
- $\log P = A - B/(C + T/K)$ (3)
- $\log P = A - B/(T/K) - C\log(T/K)$ (4)

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ΔH_v/(kJ mol⁻¹) for temp range:
- at bp 49.534
- at 25°C 73.931
eq. 2 P/mmHg

A 7.11767
B 1566.029
C 167.680

FIGURE 14.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for p-cresol.

TABLE 14.1.1.4.3
Reported Henry’s law constants of m-cresol at various temperatures and temperature dependence equations

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

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

\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3) \quad \log H = A - B/(T/K) \quad (4a)
\]

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

Dohnal & Fenclová 1995

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Feigenbrugel et al. 2004

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(Continued)
### TABLE 14.1.1.4.3 (Continued)

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<td>$calculated from eq. 3</td>
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<td>*data from literature</td>
<td>293.15</td>
<td>0.0627 *</td>
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| eq. 1 | K_{aw} | 293.15 | 0.0606 |
| A     | 9.328  | 293.15 | 0.0563 |
| B     | 5865   | 293.25 | 0.0602 |
|       |        | 298.15 | 0.0943 |
| enthalpy of hydration: | 298.25 | 0.0875 |
| ΔH_f/(kJ mol⁻¹) = 48.8 ± 0.6 | 293 | 0.0582 |
| OR | 298 | 0.0989 |

| eq. 3 | k_r/kPa | 22.071 |
| A     | 6138   |       |
| ΔH_r/(kJ mol⁻¹) = 51.0 ± 0.6 |

**FIGURE 14.1.1.4.3** Logarithm of Henry's law constant versus reciprocal temperature for p-cresol.

---

**p-Cresol: Henry's law constant vs. 1/T**

- Dohnal & Fenclová 1995
- Feigenbrugel et al. 2004

14.1.1.5 2,3-Dimethylphenol

Common Name: 2,3-Dimethylphenol
Synonym: 2,3-xylenol, 1-hydroxy-2,3-dimethylbenzene
Chemical Name: 2,3-dimethylphenol
CAS Registry No: 526-75-0
Molecular Formula: C₈H₁₀O, CH₃C₆H₃(CH₃)OH
Molecular Weight: 122.164
Melting Point (°C):
72.5 (Lide 2003)
Boiling Point (°C):
216.9 (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
10.54 (Dohnal & Fenclová 1995)
Molar Volume (cm³/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
84.08, 47.32 (25°C, normal boiling point, Andon et al. 1960)
Enthalpy of Sublimation, ΔHₛᵤₐₙ (kJ/mol):
Entropy of Fusion, ΔSₕᵤₐₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕᵤₐₙ = 56 J/mol K), F: 0.342 (mp at 72.5°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):
40000* (150 °C, shake flask-optical method, measured range 150–208.8 °C, Erichsen & Dobbert 1955)
3930 (20 °C, shake flask or batch contacting technique-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
133.3* (56°C, summary of literature data, temp range 56–219.0°C, Stull 1947)
1333* (84.0 °C, ebulliometry, measured range 84.0–219.0 °C, Vonterres et al. 1955)
log (P/mmHg) = 13.1606 – 4389.99/(t/°C + 273); temp range 10–50°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = 7.04268 – 1069.164/(t/°C + 169.744); temp range 149–219°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/kPa) = 6.13887 – 1588.200/(167.385 + t°C); temp range 149–218°C (Antoine eq. derived from experimental data of Andon et al. 1960, Boublík et al. 1984)
log (P/kPa) = 6.01592 – 1644.433/(192.286 + t°C), temp range 84–219°C (Antoine eq. derived from experimental data of Vonterres et al. 1955, Boublík et al. 1984)
log (Pₜ/kPa) = 12.29616 – 4394.694/(T/K); temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (Pₜ/kPa) = 6.17998 – 1619.086/(–102.197 + T/K); temp range 433–492 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 82.92733 – 6.0367 × 10³/(T/K) –26.948·log (T/K) + 9.739 × 10⁻³(T/K) + 2.5196 × 10⁻¹²(T/K)²; temp range 346–723 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
0.0631, 0.0952 (20, 25°C, calculated-limiting activity coefficient γ∞ data, Dohnal & Fenclová 1995)
2.96, 5.656, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

\[ \ln K_{\text{AW}} = 11.858 - \frac{6567}{T/\text{K}}; \text{ temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995) } \]

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

2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

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, \( t_{\frac{1}{2}} \) or Lifetimes, \( \tau \):

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**TABLE 14.1.1.5.1**

Reported aqueous solubilities of 2,3-dimethylphenol at various temperatures

Erichsen & Dobbert 1955

shake flask-optical method
FIGURE 14.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylphenol.

TABLE 14.1.1.5.2
Reported vapor pressures of 2,3-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

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

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At 25°C: 84.015
At bp: 47.32

For eq. 2 P/mmHg:
A = 7.04268
B = 1609.184
C = 169.774
14.1.1.6 2,4-Dimethylphenol

Common Name: 2,4-Dimethylphenol
Synonym: 2,4-xylene, as-m-xylene, 1-hydroxy-2,4-dimethylbenzene
Chemical Name: 2,4-dimethylphenol
CAS Registry No: 105-67-9
Molecular Formula: C₈H₁₀O, CH₃C₆H₃(CH₃)OH
Molecular Weight: 122.164
Melting Point (°C):
  24.5 (Lide 2003)
Boiling Point (°C):
  210.98 (Lide 2003)
Density (g/cm³ at 20°C):
  1.0202 (Andon et al. 1960)
  0.9650 (Weast 1982–83)
Molar Volume (cm³/mol):
  147.8 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
  10.60 (Herigton & Kynaston 1957; quoted, Callahan et al. 1979)
  10.58 (Dean 1985)
  10.63 (Riddick et al. 1986; Howard 1989)
  10.10 (Kollig 1993)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  47.15 (at normal boiling point, Andon et al. 1960)
  65.86 (at 25°C, Andon et al. 1960; Dean 1992)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 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):
  8795 (shake flask-UV at pH 5.1, Blackman et al. 1955)
  6200 (shake flask-UV at pH 6.5, Blackman et al. 1955)
  6200* (synthetic method/shake flask-optical, extrapolated value, measured range 160–213.5°C, Ericksen & Dobbert 1955)
  7868 (shake flask-LSC, Banerjee et al. 1980)
  7888 (shake flask-radioactive analysis, Veith et al. 1980)
  7819 (generator column-HPLC, Wasik et al. 1981)
  8200 (shake flask-HPLC/UV, Varhaníčková 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):
  133.3* (51.8°C, summary of literature data, temp range 51.8–211.0°C, Stull 1947)
  21.78 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.37688 – 1838.9/(1999.0 + t°C); temp range 115–245°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = 10.5277 – 3439.99/(t/°C + 273); temp range 9–45°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

log (P/mmHg) = 7.04694 – 1581.391/(t/°C + 168.652); temp range 114–212°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)

log (P/mmHg) = –0.2185 × 1310.2/(T/K) + 8.867260; temp range 51.8–211.5°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = [0.2185 × 1310.2/(T/K) – 8.867260]; temp range 114–212°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)

log (P/mmHg) = 7.05539 – 1587.459/(169.437 + t/°C); temp range 89.5–211°C (Antoine eq. from reported exptl. data of Vontelles et al. 1955, Boublik et al. 1984)

log (P/mmHg) = 6.1672 – 1578.685/(–104.772 + T/K); temp range 429–486 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/L/kPa) = 6.1672 – 1578.685/(–104.772 + T/K); temp range 429–486 K (Antoine eq.-II, Stephenson & Malanowski 1987)

ln [H/(atm m3/mol)] = –16.34 – 3307/(T/K), temp range 10–30 °C (EPICS measurements, Ashworth et al. 1988)

ln KAW = 10.077 – 5811/(T/K); temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

ln KAW = 10.077 – 5811/(T/K); temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

ln KAW = 10.077 – 5811/(T/K); temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

ln KAW = 10.077 – 5811/(T/K); temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)

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):

1.722 (calculate-P/C, Mabey et al. 1982)

500 (EPICS-GC, Ashworth et al. 1988)

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

ln [H/(atm m3/mol)] = –16.34 – 3307/(T/K), temp range 10–30 °C (EPICS measurements, Ashworth et al. 1988)

0.0638 (8 °C, Leuenberger et al. 1985)

0.203, 0.0692 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)

0.1815 (calculated-P/C, Shiu et al. 1994)

0.199* (calculated-limiting activity coeff. γ∞ data, Dohnal & Fenclová 1995)

4.338, 7.491, 11.46 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

0.202* (extrapolated-vapor pressure eq., Nesterova et al. 1990)

0.154 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

643 (20°C, selected from literature experimentally measured data - poor correlation coefficient, Stauffer & Roberts 2001)

log KAW = –5.192 + 1563/(T/K); poor correlation coefficient (van’t Hoff eq. derived from literature data, Stauffer & Roberts 2001)

Octanol/Water Partition Coefficient, log KOW:

2.30 (20°C, shake flask-UV, Korenman 1973)

2.42 (23 ± 1.5°C, shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)
Phenolic Compounds

2.30 (shake flask, Korenman et al. 1980)
1.99, 2.54 (RP-HPLC-RT correlation, quoted calculated value, Veith et al. 1980)
2.54 (35°C, shake flask-UV, Rogers & Wong 1980)
2.34 (generator column-HPLC, Wasik et al. 1981)
2.37 (calculated-activity coeff. $\gamma$ from UNIFAC not considering mutual solubility of octanol and water, Arbuckle 1983)
2.95 (calculated-activity coeff. $\gamma$ from UNIFAC by considering mutual solubility of octanol and water, Arbuckle 1983)
2.14 (HPLC-k’ correlation, Haky & Young 1984)
1.83 (calculated-activity coeff. $\gamma$ from UNIFAC, Banerjee & Howard 1988)
2.35 (recommended, Sangster 1989, 1993)
2.48 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
2.30 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
1.18 (bluegill sunfish, Barrows et al. 1980)
2.18 (bluegill sunfish, Veith et al. 1980)
1.86 (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)
1.88 (calculated-MCI $\chi$, Sabljic 1987a)

Sorption Partition Coefficient, log $K_{OC}$:
1.98 (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
2.63 (soil, calculated-$K_{OW}$, Lyman et al. 1982)
2.19 (activated carbon, Blum et al. 1994)
1.76 (calculated-$K_{OW}$, Kollig 1993)
2.62, 2.77 (average values for sediments, soils, Delle Site 2001)

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

Volatilization:

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_D$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k < 4 \times 10^6$ M$^{-1}$ h$^{-1}$ for singlet oxygen, 1.1 $\times 10^6$ M$^{-1}$ h$^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
photooxidation $t_1/2 = 77-3840$ h in water, based on reported reaction rate constants for RO$_2$ radicals with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991)
photooxidation $t_1/2 = 8.0$ h in air, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; selected, Howard 1989)
$k_{OH} = 7.15 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K (Atkinson 1989)
photooxidation $t_1/2 = 1.19-11.9$ h, based on estimated rate constant for the reaction with OH radical in air (Howard et al. 1991)

Hydrolysis:
Biodegradation: average rate of biodegradation 28.2 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); first-order rate constant $k = 1.0$ d$^{-1}$ corresponding to $t_1/2 = 0.7$ d in adapted activated sludge under aerobic conditions (Mills et al. 1982);

$t_{1/2}(aq. aerobic) = 24-168$ h, based on aqueous aerobic screening test data (Petrasek et al. 1983; Chambers et al. 1963; selected, Howard et al. 1991); $t_{1/2}(aq. anaerobic) = 96-672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
average $k_{exptl.} = 0.0578$ h$^{-1}$ compared to group contribution method predicted $k = 0.0758$ h$^{-1}$ (nonlinear) and $k = 0.0646$ h$^{-1}$ (linear) (Tabak & Govind 1993).
Biotransformation: rate constant for bacterial transformation of $1 \times 10^7$ 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: $t_{1/2}$ = 8.0 h, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); photooxidation $t_{1/2}$ = 1.19–11.9 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).
Surface water: photooxidation $t_{1/2}$ = 77–3840 h in water, based on reported reaction rate constants for RO$_2$ radical with the phenol class (Mill & Mabey 1985; quoted, Howard et al. 1991).
Groundwater: $t_{1/2}$ = 48–336 h, based on estimated 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).

Biotransformation:

### TABLE 14.1.1.6.1

Reported aqueous solubilities and Henry's law constants of 2,4-dimethylphenol at various temperatures

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<td>213</td>
<td>279000</td>
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<td>25</td>
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extrapolated
**Phenolic Compounds**

**FIGURE 14.1.1.6.1** Logarithm of Henry's law constant versus reciprocal temperature for 2,4-dimethylphenol.

**TABLE 14.1.1.6.2**
Reported vapor pressures of 2,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

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<td><strong>t/°C</strong></td>
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<td>$t / ^\circ C$</td>
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</table>

| $\Delta H_v / (\text{kJ mol}^{-1})$ | 211.453 | 102666 |
| at $25 ^\circ C$                  | 65.856  | 211.888 | 103803 |
| at bp                             | 47.145  | 212.32  | 106266 |

for temp range:

- 144–212°C

**eq. 2**

- P/mmHg
- A = 7.04694
- B = 1581.391
- C = 168.652

### FIGURE 14.1.1.6.2

Logarithm of vapor pressure versus reciprocal temperature for 2,4-dimethylphenol.

![Graph of vapor pressure vs. reciprocal temperature](image-url)
14.1.1.7 2,5-Dimethylphenol

[Chemical structure]

Common Name: 2,5-Dimethylphenol
Synonym: 2,5-xylene, 1-hydroxy-2,5-dimethylbenzene
Chemical Name: 2,5-dimethyl phenol
CAS Registry No: 95-87-4
Molecular Formula: C₈H₁₀O, CH₃C₆H₄(CH₃)OH
Molecular Weight: 122.164
Melting Point (°C):
  74.8 (Lide 2003)
Boiling Point (°C):
  211.1 (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
  10.41 (Dohnal & Fenclová 1995)
Molar Volume (cm³/mol):
  147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
  84.98, 46.94 (25°C, normal bp, Andon et al. 1960)
Enthalpy of Sublimation, ΔHₛᵤₜ (kJ/mol):
Enthalpy of Fusion, ΔHₜₜ (kJ/mol):
Entropy of Fusion, ΔSₜₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₜ = 56 J/mol K), F:
  0.325 (mp at 74.8°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  3126 (shake flask-UV, pH 5.1, Blackman et al. 1955)
  3122 (20°C, shake flask-UV, Dohnal & Fenclová 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):
  133.3* (51.8°C, summary of literature data, temp range 51.8–211.5°C, Stull 1947)
  1333* (89.4°C, ebulliometry, measured range 89.40–211.2°C, Vонтеррес et al. 1955)
  1.213* (24.82°C, ebulliometry/gas saturation, measured range 9.5–45°C, Andon et al. 1960)
log (P/mmHg) = 13.3705 – 4438.56/(t/ °C + 273); temp range 9–50°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = 7.03684 – 1581.906/(t/ °C + 169.497); temp range 143–212°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/kPa) = 6.1332 – 1560.465/(176.024 + t/°C), temp range 144–211.2°C (Antoine eq. derived from exptl data of Andon et al. 1960, Boublík et al. 1984)
log (P/kPa) = 6.04303 – 1383.881/(157.333 + t/°C); temp range 89.4–211.2°C (Antoine eq. derived from exptl data of Vонтеррес et al. 1955, Boublík et al. 1984)
log (P/kPa) = 12.51064 – 3950.681/(T/K), temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.17702 – 1593.804/(–102.241 + T/K); temp range 427–485 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 47.5888 – 4.8102 × 10³/(T/K) – 13.186 log (T/K) – 1.0208 × 10⁹/(T/K) + 2.7045 × 10⁻¹²(T/K)²; temp range 348–707 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0873, 0.133 (20, 25°C, calculated-limiting activity coefficient γ∞ data, Dohnal & Fenclová 1995)
- 4.353, 7.476, 11.20 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
- \( \ln K_{AW} = 12.004 - 6511/(T/K) \); temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

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

- 2.34 (shake flask, Korenman 1973)
- 2.33 (shake flask, Korenman et al. 1980)
- 2.35 (generator column-HPLC, Wasik et al. 1981)
- 2.34 (recommended, Sangster 1993)
- 2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

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

Bioconcentration Factor, log \( BCF \) or log \( K_B \):

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

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{½} \):

Half-Lives in the Environment:

---

**TABLE 14.1.1.7.1**

Reported vapor pressures of 2,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

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</tr>
</thead>
<tbody>
<tr>
<td>204.6</td>
<td>86659</td>
<td>206.8</td>
<td>93325</td>
<td>211.2</td>
<td>101325</td>
<td>eq. 2</td>
<td>P/mmHg</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>210.117</td>
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<td></td>
<td>211.736</td>
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</table>

<table>
<thead>
<tr>
<th>∆Hv/(kJ mol⁻¹) for temp range:</th>
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<tbody>
<tr>
<td>at 25°C 84.98</td>
</tr>
<tr>
<td>at bp eq. 2 P/mmHg</td>
</tr>
<tr>
<td>A 7.03684</td>
</tr>
<tr>
<td>B 1581.906</td>
</tr>
<tr>
<td>C 169.497</td>
</tr>
</tbody>
</table>

**FIGURE 14.1.1.7.1** Logarithm of vapor pressure versus reciprocal temperature for 2,5-dimethylphenol.
14.1.1.8 2,6-Dimethylphenol

Common Name: 2,6-Dimethylphenol
Synonym: 2,6-xylenol, vic-m-xylenol
Chemical Name: 2,6-dimethylphenol
CAS Registry No: 576-26-1
Molecular Formula: C₈H₁₀O, CH₃C₆H₃(CH₃)OH
Molecular Weight: 122.164
Melting Point (°C):
45.8 (Lide 2003)
Boiling Point (°C):
201.07 (Lide 2003)
Density (g/cm³ at 20°C):
1.1320 (25°C, Andon et al. 1960)
Molar Volume (cm³/mol):
107.9 (25°C, calculated-density)
147.8 calculated-Le Bas method at normal boiling point
Acid Dissociation Constant, pKₐ:
10.60 (McLeese et al. 1979; Dean 1985; Varhaníčková et al. 1995)
10.63 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
60.41, 46.97 (25°C, bp, Dreisbach 1955)
44.52 (at normal boiling point, Andon et al. 1960)
Enthalpy of Sublimation, ΔHₘₙₜ (kJ/mol):
75.6 (at 25°C, Andon et al. 1960; Dean 1992)
Enthalpy of Fusion, ΔHₚₑₑₙ (kJ/mol):
18.9; 16.3 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔSₚₑₑₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₑₑₙ = 56 J/mol K.), F: 0.625 (mp at 45.8°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):
6230 (shake flask-UV at pH 5.1, Blackman et al. 1955)
13000* (130 °C, shake flask-optical method, measured range 130–241.2°C, Erichsen & Dobbert 1955)
9650 (generator column-HPLC, Wasiš et al. 1981)
2900, 5900 (8, 25°C, Leuenberger et al. 1985)
9560 (20°C, shake flask-UV, Dohnal & Fenclová 1995)
6150 (shake flask-HPLC/UV at pH 6.3, Varhaníčková 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):
19.086 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.40318 – 1858.7/(199.0 + t/°C); temp range 115–250°C (Antoine eq. for liquid state, Dreisbach 1955)
1333* (92.5°C, ebulliometry, measured range 92.5–212.0°C, Vonterrès et al. 1955)
23.3* (24.67°C, ebulliometric and gas-saturation methods, measured range 4.75–40°C, Andon et al. 1960)
24.31 (calculated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)
log (P/mmHg) = 12.5036 – 3948.27/(t/°C + 273); temp range 4–40°C (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = 7.05753 – 1618.528/(t/°C + 186.482); temp range 144–203°C (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)
Phenolic Compounds

34.41 (extrapolated-Antoine eq., Boublik et al. 1973)
\[
\log (P/\text{mmHg}) = 7.0707 - 1628.323/(187.603 + t/\degree\text{C}), \text{ temp range } 144.8-203.5 \degree\text{C} \text{ (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)}
\]

33.68 (extrapolated-Cox eq., Chao et al. 1983)
\[
\log (P/\text{mmHg}) = [1- 474.112/(T/\text{K})] \times 10^{0.99333 - 9.96552 \times 10^{-4} T/\text{K} + 8.34247 \times 10^{-7} (T/\text{K})^2}; \text{ temp range } 321.81-701.65 \text{K} \text{ (Cox eq., Chao et al. 1983)}
\]

34.41, 10.37 (extrapolated-Antoine eq., Boublik et al. 1984)
\[
\log (P/\text{mmHg}) = 6.19572 - 1628.413/(187.613 + t/\degree\text{C}), \text{ temp range } 144.8-203.5 \degree\text{C} \text{ (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)}
\]

34.41, 10.37, 9.7 (extrapolated-Antoine eq., Boublik et al. 1984)
\[
\log (P/\text{mmHg}) = 6.57979 - 1831.266/(188.83 + t/\degree\text{C}), \text{ temp range } 97.5-212 \degree\text{C} \text{ (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

34.4 (extrapolated-Antoine eq., Dean 1985)
\[
\log (P/\text{mmHg}) = 7.00707 - 1628.32/(187.60 + t/\degree\text{C}); \text{ temp range } 145-204 \degree\text{C} \text{ (Antoine eq., Dean 1985, 1992)}
\]

19.09 (selected, Riddick et al. 1986)

24.0 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\[
\log (P/\text{atm}) = 11.6308 - 3950.681/(T/\text{K}); \text{ temp range } 277-313 \text{K} \text{ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)}
\]

43.8 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
\[
\log (P/\text{Pa}) = 39.83138 - 4062.725/(T/\text{K}) - 10.16994 \log (T/\text{K}) + 0.20170 \times 10^{-2} (T/\text{K}) + 2.2316 \times 10^{-12} (T/\text{K})^2; \text{ temp range } 319-701 \text{K} \text{ (vapor pressure eq., Yaws 1994)}
\]

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

0.684 (modified gas-stripping, Hawthorne et al. 1985)

0.193 (8°C, Leuenberger et al. 1985)

0.377 (calculated-P/C, Shiu et al. 1994)

0.302 (calculated-activity coeff. γ∞ data, Dohnal & Fenclová 1995)

10.3, 17.81, 25.2 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

0.441 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
\[
\ln K_{\text{AW}} = 11.176 - 5906/(T/\text{K}), \text{ temp range } 20-100 \degree\text{C} \text{ (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)}
\]

0.098 (calculated-group contribution, Lee et al. 2000)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:

2.36 (Leo et al. 1971; Hansch & Leo 1979)

2.34 (LC-K′ correlation; Carlson et al. 1975)

2.40 (35°C, shake flask-UV, Rogers & Wong 1980)

2.31 (generator column-HPLC, Wasik et al. 1981)

2.07 (HPLC-K′ correlation, Haky & Young 1984)

2.51 (HPLC-RT correlation, Eadsforth 1986)

2.36 (recommended, Sangster 1989, 1993)

2.36 (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_1/2:

Volatilization:

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

\[
k_{\text{OH}} = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K (Atkinson 1989)}
\]

\[
k_{\text{OH}}(\text{calc}) = 54.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ estimated from Atmospheric Oxidation Program, } \kappa_{\text{OH}}(\text{exptl}) = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } k_{\text{OH}}(\text{calc}) = 30.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ estimated from Fate of Atmospheric Pollutants Program (Meylan & Howard 1993)}
\]

\[
k_{\text{OH}}(\text{calc}) = 49.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital estimation method, Klamt 1993)}
\]

Hydrolysis:

Biodegradation: \( t_{1/2} = 7–10 \text{ d} \) for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964); average rate of biodegradation 9.0 mg COD g\(^{-1}\) h\(^{-1}\) based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

Biotransformation:

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

### TABLE 14.1.1.8.1

Reported aqueous solubilities and vapor pressures of 2,6-dimethylphenol at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Erichsen &amp; Dobbert 1955</strong></td>
<td><strong>Vonterres et al. 1955</strong></td>
</tr>
<tr>
<td><strong>shake flask-optical method</strong></td>
<td><strong>ebulliometry</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
</tr>
<tr>
<td>130</td>
<td>13000</td>
</tr>
<tr>
<td>140</td>
<td>16000</td>
</tr>
<tr>
<td>150</td>
<td>21000</td>
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<tr>
<td>160</td>
<td>27000</td>
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<td>36000</td>
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<td>220</td>
<td>120000</td>
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<td>176000</td>
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<td>232</td>
<td>191000</td>
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<td>209000</td>
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<td>238</td>
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<td>240</td>
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</tr>
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<td>241.2</td>
<td>440000</td>
</tr>
<tr>
<td>212.0</td>
<td>101325</td>
</tr>
<tr>
<td>( \Delta H_v/(kJ \text{ mol}^{-1}) )</td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>75.60</td>
</tr>
<tr>
<td>at bp</td>
<td>44.52</td>
</tr>
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</table>
TABLE 14.1.1.8.1  (Continued)

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
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<tbody>
<tr>
<td>Erichsen &amp; Dobbert 1955</td>
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<td>shake flask-optical method</td>
<td>ebulliometry</td>
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<table>
<thead>
<tr>
<th>t /°C</th>
<th>S /g·m⁻³</th>
<th>t /°C</th>
<th>P /Pa</th>
<th>t /°C</th>
<th>P /Pa</th>
<th>t /°C</th>
<th>P /Pa</th>
</tr>
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<td></td>
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</tbody>
</table>

for temp range: 144–203°C

eq. 2  
P/mmHg  
A 7.05753  
B 1618.528  
C 186.492

FIGURE 14.1.1.8.1  Logarithm of vapor pressure versus reciprocal temperature for 2,6-dimethylphenol.
14.1.1.9 3,4-Dimethylphenol

Common Name: 3,4-Dimethylphenol  
Synonym: 3,4-xylene, as-o-xylene  
Chemical Name: 3,4-dimethylphenol  
CAS Registry No: 95-65-8  
Molecular Formula: C₈H₁₀O, CH₃C₆H₃(CH₃)OH  
Molecular Weight: 122.164  
Melting Point (°C):  
65.1 (Lide 2003)  
Boiling Point (°C):  
227 (Lide 2003)  
Density (g/cm³ at 20°C):  
1.1380 (25°C, Andon et al. 1960)  
0.9830 (Weast 1982–83)  
Molar Volume (cm³/mol):  
147.8 (calculated-Le Bas method at normal boiling point)  
Acid Dissociation Constant, pKₐ:  
10.40 (McLeese et al. 1979)  
10.32 (Dean 1985)  
10.36 (Riddick et al. 1986)  
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):  
49.67 (at normal boiling point, Andon et al. 1960)  
Enthalpy of Sublimation, ΔHₛₐᵤₐ (kJ/mol):  
85.73 (at 25°C, Andon et al. 1960; Dean 1992)  
Enthalpy of Fusion, ΔHₚₜₜ (kJ/mol):  
18.13; 17.0 (exptl.; calculated-group additivity method, Chickos et al. 1999)  
Entropy of Fusion, ΔSₚₜₜ (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSₚₜₜ = 56 J/mol K), F: 0.404 (mp at 65.1°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):  
5100 (shake flask-UV, Blackman et al. 1955)  
5100* (synthetic method/shake flask-optical, extrapolated value, measured range 130–190.2°C, Ericksen & Dobbert 1955)  
5000 (shake flask-spectrophotometry, Roberts et al. 1977)  
12810 (20°C, shake flask-UV, Dohnal & Fenclová 1995)  
7250 (shake flask-HPLC/UV at pH 6.25, Varhaníčková 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):  
133.3* (66.2°C, summary of literature data, temp range 66.2–225.2°C, Stull 1946)  
5.160 (calculated-Antoine eq., Dreisbach 1955)  
log (P/mmHg) = 7.70494 – 2030.9/(196.0 + t°C); temp range 130–265°C (Antoine eq. for liquid state, Dreisbach 1955)
Phenolic Compounds

1333* (105.7 °C, ebulliometry, measured range 105.7–226.0°C, Vonterres et al. 1955)
1.895 (interpolated-Antoine eq. from ebulliometric/gas-saturation measurements, Andon et al. 1960)
\[
\log (P/\text{mmHg}) = 13.1729 - 4478.23/(t/°C + 273); \text{ temp range: } 9–50°C, \text{ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)}
\]
\[
\log (P/\text{mmHg}) = 7.07343 - 1617.202/(t/°C + 158.778); \text{ temp range } 171–229°C \text{ (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)}
\]
\[
\log (P/\text{mmHg}) = [–0.2185 × 1399.10/(T/K)] + 9.02680; \text{ temp range } 66.2–225.2°C \text{ (Antoine eq., Weast 1972–73)}
\]
\[
2.541 \text{ (extrapolated-Antoine eq., Boublík et al. 1973)}
\]
\[
\log (P/\text{mmHg}) = 7.07979 – 1621.451/(159.261 + t/°C); \text{ temp range } 172–228°C \text{ (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublík et al. 1973)}
\]
3.621 \text{ (extrapolated-Cox eq., Chao et al. 1983)}
\[
\log (P/\text{mmHg}) = 12.31521 – 4485.317/(T/K); \text{ temp range } 445–502 \text{ K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{mmHg}) = 6.20617 – 1623.592/(–113.623 + T/K); \text{ temp range } 20–100 \text{ °C (vapor-liquid equilibrium VLE measurements with additional lit. data, Dohnal & Fenclová 1995)}
\]
\[
3.795 \text{ (extrapolated-four parameter vapor pressure eq., Nesterova et al. 1990)}
\]
\[
\log (P/\text{mmHg}) = 93.28460 – 6735.317/(T/K) – 29.48566·\log (T/K) + 0.95432 × 10^{–2}·(T/K)^2; \text{ temp range: } 445–502 \text{ K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1950, Nesterova et al. 1990)}
\]
\[
\log (P/\text{mmHg}) = 68.6521 – 6.15 × 10^{3}/(T/K) – 20.184·\log (T/K) – 1.1259 × 10^{–10}·(T/K) + 4.0266 × 10^{–6}·(T/K)^2; \text{ temp range } 338–730 \text{ K (vapor pressure eq., Yaws 1994)}
\]

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

0.00942 \text{ (Leuenberger et al. 1985)}
0.0212 \text{ (calculated-P/C, Shiu et al. 1994)}
0.0278 \text{ (20°C, calculated-activity coeff. γ∞ data, Dohnal & Fenclová 1995)}
1.416, 2.903, 4.619 \text{ (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)}
0.0421 \text{ (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)}
\ln K_{AW} = 11.854 – 6809/(T/K), \text{ temp range } 20–100°C \text{ (vapor-liquid equilibrium VLE measurements with additional lit. data, Dohnal & Fenclová 1995)}
0.098 \text{ (calculated-group contribution, Lee et al. 2000)}

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

2.23 \text{ (20°C, shake flask-UV, Korenman 1973)}
2.23 \text{ (shake flask, Korenman et al. 1980)}
2.23 \text{ (recommended, Sangster 1989, 1993)}
2.23 \text{ (recommended, Hansch et al. 1995)}
2.36 \text{ (HPLC-RT correlation, Makovskaya et al. 1995b)}
2.26 \text{ (solid-phase micro-extraction, Dean et al. 1996)}

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:

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:

$k_{OH} = 81.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 55.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital estimation method, Klamt 1993)

Biodegradation: average rate of biodegradation 13.4 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

### TABLE 14.1.1.9.1
**Reported aqueous solubilities of 3,4-dimethylphenol at various temperatures**

Erichsen & Dobbert 1955

<table>
<thead>
<tr>
<th>°C</th>
<th>CS / g·m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>130</td>
<td>29000</td>
</tr>
<tr>
<td>140</td>
<td>36000</td>
</tr>
<tr>
<td>150</td>
<td>42000</td>
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<tr>
<td>160</td>
<td>59000</td>
</tr>
<tr>
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<td>81000</td>
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<td>124000</td>
</tr>
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</tr>
<tr>
<td>188</td>
<td>200000</td>
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<td>189</td>
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</tr>
<tr>
<td>190</td>
<td>278000</td>
</tr>
<tr>
<td>190.2</td>
<td>336000</td>
</tr>
<tr>
<td>25</td>
<td>5100*</td>
</tr>
</tbody>
</table>

*extrapolated

### TABLE 14.1.1.9.2
**Reported vapor pressures of 3,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations**

**Stull 1947**

<table>
<thead>
<tr>
<th>°C</th>
<th>CP / Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>66.2</td>
<td>133.3</td>
</tr>
<tr>
<td>93.8</td>
<td>666.6</td>
</tr>
<tr>
<td>107.7</td>
<td>1333</td>
</tr>
</tbody>
</table>

**Vonterres et al. 1955**

<table>
<thead>
<tr>
<th>°C</th>
<th>CP / Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>105.7</td>
<td>1333</td>
</tr>
<tr>
<td>125.8</td>
<td>3333</td>
</tr>
<tr>
<td>142.6</td>
<td>6666</td>
</tr>
</tbody>
</table>

**Andon et al. 1960**

<table>
<thead>
<tr>
<th>°C</th>
<th>CP / Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.89</td>
<td>0.293</td>
</tr>
<tr>
<td>14.78</td>
<td>0.543</td>
</tr>
<tr>
<td>19.98</td>
<td>1.031</td>
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<td>171.933</td>
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<td>186.548</td>
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(Continued)
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<th>Stull 1947</th>
<th>Vonterres et al. 1955</th>
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<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
</tr>
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<td>193.9</td>
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<td>225.2</td>
<td>101325</td>
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<tr>
<td>198.7</td>
<td>46663</td>
<td>mp/°C</td>
</tr>
<tr>
<td>203.0</td>
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<td>b.p./°C</td>
</tr>
<tr>
<td>212.5</td>
<td>66661</td>
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<td>213.4</td>
<td>73327</td>
<td>for temp range:</td>
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<tr>
<td>216.5</td>
<td>79993</td>
<td>9–50°C</td>
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<tr>
<td>219.2</td>
<td>86659</td>
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</tr>
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<td>222.0</td>
<td>93325</td>
<td>A</td>
</tr>
<tr>
<td>226.0</td>
<td>101325</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
</tr>
<tr>
<td>Δ$H_v$(kJ mol$^{-1}$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>85.73</td>
<td></td>
</tr>
<tr>
<td>at b.p</td>
<td>49.67</td>
<td>171–229°C</td>
</tr>
</tbody>
</table>

$\Delta H_v$ (kJ mol$^{-1}$) at 25°C

$\Delta H_v$ (kJ mol$^{-1}$) at b.p.

FIGURE 14.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 3,4-dimethylphenol.
14.1.1.10 3,5-Dimethylphenol

Common Name: 3,5-Dimethylphenol
Synonym: 3,5-xylenol, 1-hydroxy-3,5-dimethylbenzene
Chemical Name: 3,5-dimethyl phenol
CAS Registry No: 108-68-9
Molecular Formula: C8H10O
CH₃C₆H₃(CH₃)OH
Molecular Weight: 122.164
Melting Point (°C):
63.4 (Lide 2003)
Boiling Point (°C):
221.74 (Lide 2003)
Density (g/cm³):
Acid Dissociation Constants, pKₐ:
7.8 (McLeese et al. 1979)
10.19 (Dohnal & Fenclová 1995)
Molar Volume (cm³/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
82.84, 49.31 (25°C, normal bp, Andon et al. 1960)
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.420 (mp at 63.4°C)
Water Solubility (g/m³ or mg/L at 25°C):
4886 (shake flask-UV, pH 5.1, Blackman et al. 1955)
4425 (20°C, shake flask-UV, Dohnal & Fenclová 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):
133.3* (62.0°C, summary of literature data, temp range 62–219.5°C, Stull 1947)
1333* (102.8°C, ebulliometry, measured range 102.8–219.0°C, Vonteres et al. 1960)
log (P/mmHg) = 12.8271 – 4328.13/(t/°C + 273); temp range 9–50°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/kPa) = 6.25752 – 1641.206/(164.311 + t/°C), temp range 154.7–223.3°C (Antoine eq. derived from reported exptrl data of Andon et al. 1960, Boublik et al. 1984)
log (P/mmHg) = 8.27972 – 3182.232/(287.862 + t/°C), temp range 102.8–219°C (Antoine eq. derived from reported exptrl data of Vonteres et al. 1960, Boublik et al. 1984)
log (P/kPa) = 11.97153 – 4336.025/(T/K); temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.25292 – 1638.564/(-109.095 + T/K); temp range 427–497 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = -44.915 – 2.8912 × 10⁵/(T/K) + 25.704·log (T/K) – 3.9714 × 10⁻²·(T/K) + 1.6464 × 10⁻⁵·(T/K)²; temp range 337–716 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

0.0419, 0.0614 (20, 25°C, calculated-limiting activity coefficient γ∞ data, Dohnal & Fenclová 1995)
1.95, 3.70, 6.12 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
ln KAW = 11.654 – 6636/(T/K); temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, log KW:

2.31 (shake flask, Korenman 1972; Korenman et al. 1980)
2.55 (shake flask-UV, Rogers & Wong 1980)
2.38 (UNIFAC activity coefficient, Campbell & Luthy 1985)
2.54 (HPLC-RT correlation, Eadsforth 1986)
2.35 (shake flask, Log P Database, Hansch & Leo 1987)
2.35 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log KOA:

Bioconcentration Factor, log BCF or log Kb:

Sorption Partition Coefficient, log KOC:

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

Half-Lives in the Environment:

### TABLE 14.1.1.10.1

Reported vapor pressures of 3,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>(1) ln P = A – B/(T/K)</th>
<th>(1a) log P = A – B/(T/K)</th>
<th>(2) ln P = A – B/(C + t/°C)</th>
<th>(2a) log (P/mmHg) = A – B/(C + t/°C)</th>
<th>(3) ln P = A – B/(C + T/K)</th>
<th>(3a) log (P/mmHg) = A – B/(C + T/K) – C·log (T/K)</th>
<th>(4) log (P/mmHg) = A – B/(T/K)</th>
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<tr>
<td>62</td>
<td>133.3</td>
<td>102.8</td>
<td>13.3</td>
<td>9.57</td>
<td>0.44</td>
<td>154.72</td>
<td>12984</td>
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<tr>
<td>89.2</td>
<td>666.6</td>
<td>122.5</td>
<td>333</td>
<td>14.92</td>
<td>0.813</td>
<td>166.472</td>
<td>19760</td>
<td></td>
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<tr>
<td>102.4</td>
<td>1333</td>
<td>139.1</td>
<td>666</td>
<td>20.35</td>
<td>1.58</td>
<td>175.126</td>
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<tr>
<td>117.0</td>
<td>2666</td>
<td>149.0</td>
<td>9999</td>
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<td>5333</td>
<td>156.8</td>
<td>13332</td>
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<td>4.866</td>
<td>187.937</td>
<td>39757</td>
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<td>143.5</td>
<td>7999</td>
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<td>176.3</td>
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<td>197.8</td>
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<td>39997</td>
<td>49.97</td>
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<td>205.601</td>
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<td>191.0</td>
<td>43330</td>
<td>55.17</td>
<td>40.57</td>
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<td>212.159</td>
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<td>63.27</td>
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<td>96027</td>
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<td>211.0</td>
<td>79993</td>
<td>220.692</td>
<td>eq. 2</td>
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<td>220.097</td>
<td>97296</td>
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<td>98771</td>
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TABLE 14.1.1.10.1 (Continued)

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<td>summary of literature data</td>
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<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
<td>$t/°C$</td>
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<td>216.2</td>
<td>93325</td>
<td>A</td>
</tr>
<tr>
<td>219.0</td>
<td>101325</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Δ$H_v$/kJ mol$^{-1}$</td>
</tr>
<tr>
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</table>

For temp range: 154–224°C

eq. 2 $P/\text{mmHg}$

A | 7.11745
B | 1630.124
C | 163.076

FIGURE 14.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 3,5-dimethylphenol.
14.1.1.11 2,3,5-Trimethylphenol

Common Name: 2,3,5-Trimethylphenol
Synonym:
Chemical Name: 2,3,5-trimethylphenol
CAS Registry No: 697-82-5
Molecular Formula: C₉H₁₂O, C₆H₂(CH₃)₃OH
Molecular Weight: 136.190
Melting Point (°C):
  94.5 (Lide 2003)
Boiling Point (°C):
  233 (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
  10.60 (Blackman et al. 1955)
Molar Volume (cm³/mol):
  170.0 (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: 0.208 (mp at 94.5°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):
  40000* (200°C, synthetic method/shake flask-optical, measured range 200–248°C, Erichsen & Dobbert 1955)
  762 (shake flask-UV, Blackman et al. 1955)
  855 (shake flask-HPLC/UV at pH 5.95, Varhaníčková 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):
  2.426* (extrapolated-Antoine eq., ebulliometry, measured range 186–247°C, Handley et al. 1964)
  log (P/mmHg) = 7.08022 – 1685.973/(166.150 + t/°C); temp range 186–247°C (Antoine eq., ebullimetric method, Handley et al. 1964)
  4.451 (extrapolated-Cox eq., Chao et al. 1983)
  log (P/mmHg) = [1–508.477/(T/K)] × 10^8[0.932965 – 5.75276 × 10⁻³(T/K) + 3.29737 × 10⁻⁵(T/K)²]; temp range: 459.63–520.21 K, (Cox eq., Chao et al. 1983)
  2.426 (extrapolated-Antoine eq., Boublik et al. 1973)
  log (P/mmHg) = 7.08012 – 1685.896/(166.141 + t/°C), temp range 186.5–247°C (Antoine eq. from reported expl. data of Handley et al. 1964, Boublik et al. 1984)
  2.43, 0.0234 (extrapolated from liquid, Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 6.02493 – 1685.528/(166.133 + t/°C), temp range 186.5–247°C (Antoine eq. from reported expl. data of Handley et al. 1964, Boublik et al. 1984)
  log (P/kPa) = 6.95436 – 889.02/(67.752 + t/°C), temp range 106–233°C (Antoine eq. from reported expl. data, Boublik et al. 1984)
  2.43 (extrapolated-Antoine eq., Dean 1985)
  log (P/mmHg) = 7.08012 – 1685.90/(166.14 + t/°C), temp range 186–247°C (Antoine eq., Dean 1985, 1992)
  2.44 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)
log \( \frac{P}{Pa} \) = 89.62984 – 6541.396/(T/K) – 28.26318·log (T/K) + 0.92991 × 10^{-2}·(T/K); temp range: 460–520 K
(four-parameter vapor pressure eq. derived using exptl data of Handley et al. 1964, Nesterova et al. 1990)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.404 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
3.06 (COMPUTOX databank, Kaiser 1993)
2.92 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \):
3.61 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Half-Lives in the Environment:

TABLE 14.1.1.11.1
Reported aqueous solubilities and vapor pressures of 2,3,5-trimethylphenol at various temperatures

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<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Erichsen &amp; Dobbert 1955</td>
<td>Handley et al. 1964</td>
</tr>
<tr>
<td>shake flask-optical method</td>
<td>ebulliometry</td>
</tr>
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<td>( t/°C )</td>
<td>( S/g·m^{-3} )</td>
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<tr>
<td>200</td>
<td>40000</td>
</tr>
<tr>
<td>210</td>
<td>54000</td>
</tr>
<tr>
<td>220</td>
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<td>291000</td>
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<tr>
<td>257.8</td>
<td>420000</td>
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</tbody>
</table>

mp/°C 93.73
bp/°C 235.329
<table>
<thead>
<tr>
<th>TABLE 14.1.11.1 (Continued)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous solubility</td>
</tr>
<tr>
<td>Erichsen &amp; Dobbert 1955</td>
</tr>
<tr>
<td>shake flask-optical method</td>
</tr>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>S/g·m⁻³</td>
</tr>
</tbody>
</table>

for temp range: 186–247°C

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

<table>
<thead>
<tr>
<th>P/mmHg</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
</tr>
<tr>
<td>B</td>
</tr>
<tr>
<td>C</td>
</tr>
</tbody>
</table>

\[\Delta H_v/(kJ mol^{-1})\]

at bp 49.96
14.1.1.12 2,4,6-Trimethylphenol

Common Name: 2,4,6-Trimethylphenol
Synonym: Mesitol
Chemical Name: 2,4,6-Trimethylphenol
CAS Registry No: 527-60-6
Molecular Formula: C₉H₁₂O, C₈H₂(CH₃)₃OH
Molecular Weight: 136.190
Melting Point (°C):
  73  (Lide 2003)
Boiling Point (°C):
  220  (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
  10.90  (Blackman et al. 1955)
  10.88  (Dean 1985)
Molar Volume (cm³/mol):
  170.0  (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: 0.338 (mp at 73°C)
Water Solubility (g/m³ or mg/L at 25°C):
  1007  (shake flask-UV, Blackman et al. 1955; quoted, Varhaníčková et al. 1995)
  1420  (shake flask-HPLC/UV at pH 4.85, Varhaníčková et al. 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  7.0  (extrapolated from liquid state, Antoine eq., Boublik et al. 1984)
  19.6  (supercooled liquid P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
Log (P/Pa) = 5.91352 – 1481.329/(158.589 + t/°C), temp range 94–220.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
Henry’s Law Constant (Pa m³/mol at 25°C):
  0.2512  (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, log K_{ow}:
  2.73  (generator column-HPLC/UV, Wasik et al. 1981)
  2.73  (quoted and recommended, Sangster 1989; 1993)
  2.7  3  (COMPUTOX databank, Kaiser 1993)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, or Half-Lives, t₁/₂:
Half-Lives in the Environment:
14.1.1.13 3,4,5-Trimethylphenol

Common Name: 3,4,5-Trimethylphenol
Synonym:
Chemical Name: 3,4,5-trimethylphenol
CAS Registry No: 527-54-8
Molecular Formula: C₉H₁₂O, C₆H₂(CH₃)₃OH
Molecular Weight: 136.190
Melting Point (°C): 108 (Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C): 249 (Stephenson & Malanowski 1987)
248.5 (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
10.25 (Dean 1985)
Molar Volume (cm³/mol):
170.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25 °C (assuming ΔSfus = 56 J/mol K), F: 0.153 (mp at 108 °C)
Water Solubility (g/m³ or mg/L at 25°C):
1538 (shake flask-HPLC/UV, Varhaníčková et al. 1994)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (Pv/kPa) = 7.33216 – 2536.1/(-44.56 + T/K), temp range 396–521 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kow:
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kbi:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
14.1.1.14 \( o \)-Ethylphenol

![Chemical Structure of o-Ethylphenol](image)

Common Name: 2-Ethylphenol
Synonym: \( o \)-ethylphenol
Chemical Name: 2-ethylphenol, \( o \)-ethylphenol
CAS Registry No: 90-00-6
Molecular Formula: \( C_8H_{10}O, C_2H_5C_6H_4OH \)
Molecular Weight: 122.164
Melting Point (°C):
- 18 (Lide 2003)
Boiling Point (°C):
- 204.5 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
- 1.01885, 1.01459 (20°C, 25°C Biddiscombe et al. 1963)
- 1.0370 (Vershueren 1983; 25°C, Dean 1985)
Molar Volume (cm\(^3\)/mol):
- 117.8 (0°C, Stephenson & Malanowski 1987)
- 147.8 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, \( pK_a \):
- 10.02 (Dean 1985)
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):
- 14040 (shake flask-HPLC/UV at pH 5.2, Varhaníčková 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):
- 133.3* (46.2 °C, summary of literature data, temp range 46.2–207.5°C, Stull 1947)
- 33.66 (calculated-Antoine eq., Dreisbach 1955)
- \[ \log (P/mmHg) = 7.23343 - 1771.5/(200.0 + t/°C), \text{ temp range 105–245°C} \] (Antoine eq. for liquid state, Dreisbach 1955)
- 20.84 (interpolated-Antoine eq., Biddiscombe et al. 1963)
- 20.4* (24.93°C, ebulliometric and gas transpiration measurements, measured range 5–45°C, Biddiscombe & Martin 1958)
- \[ \log (P/mmHg) = 10.3131 - 3313.50/(t/°C + 273); \text{ temp range 5–45°C} \] (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)
- \[ \log (P/mmHg) = 7.00742 - 1648.923/(t/°C + 170.83); \text{ temp range 150–218°C} \] (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)
- \[ \log (P/mmHg) = (1 - 0.2185 \times 12516.7/(T/K)) + 8.586948; \text{ temp range 46.2–207.5°C} \] (Antoine eq., Weast 1972–73)
- \[ \log (P/mmHg) = [1 - 480.731/(T/K)] \times 10^6(0.883881 - 6.07675 \times 10^{-4}(T/K) + 6.44264 \times 10^{-7}(T/K)^2]; \text{ temp range: 319.35–480.65 K,} \] (Cox eq., Chao et al. 1983)
- 16.7, 29 (extrapolated-Antoine eq., Boublík et al. 1984)
- \[ \log (P/kPa) = 6.13214 - 1548.802/(170.82 + t/°C); \text{ temp range 150.4–215.05°C} \] (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublík et al. 1984)
- \[ \log (P/kPa) = 6.97225 - 2178.815/(231.035 + t/°C); \text{ temp range 86–207.5°C} \] (Antoine eq. from reported exptl. data of Vonterrés et al. 1955, Boublík et al. 1984)
- 27.01 (extrapolated-Antoine eq., Dean 1985)
- \[ \log (P/mmHg) = 7.8003 - 2140.4/(227 + t/°C); \text{ temp range 86–208°C} \] (Antoine eq., Dean 1985, 1992)
- 20.87 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.13344 – 1550.409/(–102.103 + T/K); temp range 423–491 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)
log (P/kPa) = 9.44878 – 3318.181/(T/K), temp range 277–318 K (Antoine eq.-II, Stephenson & Malanowski 1987)
19.55 (extrapolated-Antoine eq., Nesterova et al. 1990)
\[ \log (P/Pa) = 94.95377 – 6350.841/(T/K) – 30.56287 \cdot \log (T/K) + 1.09475 \times 10^{-2} \cdot (T/K); \text{ temp range: } 424–491 \text{ K} \] (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.174 (calculated with selected-P/C)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- 2.47 (shake flask, Hansch & Leo 1979)
- 2.64 (shake flask, Korenman 1980)
- 2.64 (HPLC-RT correlation, Butte et al. 1981)
- 2.47 (recommended, Sangster 1989, 1993)
- 2.46 (HPLC-RT correlation, Ritter et al. 1994)
- 2.47 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

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

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 14.1.1.14.1</th>
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<tbody>
<tr>
<td>Reported vapor pressures of ( \alpha )-ethylphenol at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

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

Stull 1947

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<tr>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
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<td>3.346</td>
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<tr>
<td>73.4</td>
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<td>mp/°C</td>
<td>–45</td>
<td>mp/°C</td>
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</table>

Biddiscombe et al. 1963

<table>
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<th>( t/°C )</th>
<th>( P/Pa )</th>
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(Continued)
TABLE 14.1.1.14.1 (Continued)

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<td><strong>P/Pa</strong></td>
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<tr>
<td>for temp range:</td>
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<tr>
<td>5–45°C</td>
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<tr>
<td>eq. 2</td>
<td>212.651</td>
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<tr>
<td>A</td>
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<tr>
<td>B</td>
<td>3313.50</td>
</tr>
<tr>
<td>C</td>
<td>273</td>
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<tr>
<td>∆Hv/(kJ mol⁻¹)</td>
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<tr>
<td>at 25°C</td>
<td>63.60</td>
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<tr>
<td>at bp</td>
<td>48.116</td>
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</table>

**FIGURE 14.1.1.14.1** Logarithm of vapor pressure versus reciprocal temperature for o-ethylphenol.

© 2006 by Taylor & Francis Group, LLC
Common Name: 4-Ethylphenol
Synonym: p-ethylphenol
Chemical Name: 2-ethylphenol, p-ethylphenol
CAS Registry No: 123-07-9
Molecular Formula: C₈H₁₀O, C₂H₅C₆H₄OH
Molecular Weight: 122.164
Melting Point (°C):
45  (Lide 2003)
Boiling Point (°C):
217.9  (Lide 2003)
Density (g/cm³ at 20°C):
1.054  (25°C, Biddiscombe et al. 1963)
1.011  (25°C, Dean 1985)
Molar Volume (cm³/mol):
147.8  (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
10.0  (Dean 1985)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
50.84  (at normal boiling point, Biddiscombe et al. 1963)
Enthalpy of Sublimation, ∆Hₛᵥ (kJ/mol):
80.33  (at 25°C, Andon et al. 1960)
Enthalpy of Fusion, ∆Hₓᵥ (kJ/mol):
Entropy of Fusion, ∆Sₕᵥ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕᵥ = 56 J/mol K), F: 0.636 (mp at 45°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):
24000*  (150°C, synthetic method-shake flask-optical, measured range 150–187°C, Erichsen & Dobbert 1955)
5000  (shake flask-spectrophotometry, Roberts et al. 1977)
7980  (shake flask-HPLC/UV, Varhaníčková 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):
133.3*  (59.3°C, summary of literature data, temp range 59.3–219.0°C, Stull 1947)
9.67  (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.55177 – 1943.1/(197.0 + t°C), temp range: 125–255°C, (Antoine eq. for liquid state, Dreisbach 1955)
1333*  (101.0°C, ebulliometry, measured range 101.0–218.2°C, Vonterrès et al. 1955)
5.030  (calculated-Antoine eq., Biddiscombe et al. 1963)
4.96*  (25.03°C, ebulliometric and gas transpiration measurements, measured range 5–44°C, Biddiscombe et al. 1963)
log (P/mmHg) = 12.6090 – 4183.50/(t°C + 273); temp range 5–44°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)
log (P/mmHg) = 7.01297 – 1548.923/(t°C + 156.820); temp range 171–229°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 13437.9/(T/K)] + 8.854990; \text{ temp range 59.3–219°C (Antoine eq., Weast 1972–73)}
\]

6.575 \hspace{1cm} \text{(extrapolated-Antoine eq., Boublik et al. 1984)}

\[
\log (P/\text{kPa}) = 6.13614 – 1547.614/(156.677 + t/°C), \text{ temp range 171.8–229.1°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)}
\]

6.575 \hspace{1cm} \text{(extrapolated-Antoine eq., Boublik et al. 1984)}

\[
\log (P/\text{kPa}) = 7.59041 – 2575.507/(242.273 + t/°C), \text{ temp range 101–218.2°C (Antoine eq. from reported exptl. data of Vonderres et al. 1955, Boublik et al. 1984)}
\]

7.530 \hspace{1cm} \text{(extrapolated-Antoine eq., Dean 1985)}

\[
\log (P/\text{kPa}) = 11.74364 – 4188.624/(T/K), \text{ temp range 278–317 K, (Antoine eq.-I, solid, Stephenson & Malanowski 1987)}
\]

log (P/kPa) = 6.13939 – 1550.479/(–116.1 + T/K), temp range: 444–502 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

7.530 \hspace{1cm} \text{(extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)}

\[
\log (P/\text{Pa}) = 96.72774 – 6779.787/(T/K) – 30.80658\cdot \log (T/K) + 1.101581 \times 10^{-2}\cdot (T/K) ; \text{ temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)}
\]

\[
\log (P/\text{mmHg}) = 16.9092 – 3.7255 \times 10^3/(T/K) – 1.7886\cdot \log (T/K) – 4.2275 \times 10^{-3}\cdot (T/K) + 1.8002 \times 10^{-6}\cdot (T/K)^2; \text{ temp range 318–716 K (vapor pressure eq., Yaws 1994)}
\]

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

0.132 \hspace{1cm} \text{(calculated-P/C, this work)}

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

2.75 \hspace{1cm} \text{(literature average, Leo et al. 1971)}

2.58 \hspace{1cm} \text{(shake flask-UV at pH 7.45, Umeyama et al. 1971)}

2.26 \hspace{1cm} \text{(shake flask, Korenman 1972, Korenman et al. 1980)}

2.26, 2.58 \hspace{1cm} \text{(Hansch & Leo 1979)}

2.60 \hspace{1cm} \text{(shake flask-UV, Rogers & Wong 1980)}

2.37 \hspace{1cm} \text{(HPLC-RT correlation, Butte et al. 1981)}

2.12, 2.19 \hspace{1cm} \text{(RP-HPLC-k’ correlation, Miyake & Terada 1982)}

2.59 ± 0.07; 2.58 \hspace{1cm} \text{(HPLC-RV correlation-ALPM, selected best lit. value, Garst & Wilson 1984)}

2.50 \hspace{1cm} \text{(recommended, Sangster 1989, 1993)}

2.50 \hspace{1cm} \text{(COMPUTOX databank, Kaiser 1993)}

2.40; 2.58 \hspace{1cm} \text{(pH 7.4, pH 5.6, Hansch et al. 1995)}

Bioconcentration Factor, log \( BCF \):

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

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

Half-Lives in the Environment:
TABLE 14.1.15.1
Reported aqueous solubilities of $p$-ethylphenol at various temperatures

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<th>$t/°C$</th>
<th>$S/g \cdot m^{-3}$</th>
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<td>150</td>
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<tr>
<td>160</td>
<td>30000</td>
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<tr>
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<td>45000</td>
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<td>180</td>
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<td>182</td>
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<td>184</td>
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<td>186</td>
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<td>187.1</td>
<td>395000</td>
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TABLE 14.1.15.2
Reported vapor pressures of $p$-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$

$\log (P/mmHg) = A - B/(C + t/°C)$

$\log (P/Pa) = A - B/(C + T/K)$

$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$

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<td>at 25°C</td>
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<td>171–229°C</td>
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FIGURE 14.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for \( p \)-ethylphenol.
**14.1.1.16 4-Propylphenol**

```
\[ \text{OH} \]
```

Common Name: 4-Propylphenol  
Synonym:  
Chemical Name: 4-propylphenol  
CAS Registry No: 645-56-7  
Molecular Formula: C₉H₁₂O, C₃H₇C₆H₄OH  
Molecular Weight: 136.190  
Melting Point (°C):  
  22  (West 1982–83; Lide 2003)  
Boiling Point (°C):  
  232.6  (Weast 1982–83; Lide 2003)  
Density (g/cm³ at 20°C):  
  1.009  (Weast 1982–83)  
Acid Dissociation Constant, pKₐ:  
Molar Volume (cm³/mol):  
  170.0  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, ΔHV (kJ/mol):  
Enthalpy of Sublimation, ΔHsubl (kJ/mol):  
Enthalpy of Fusion, ΔHfus (kJ/mol):  
Entropy of Fusion, ΔSfus (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
  1278  (shake flask-HPLC/UV, Varhaněková et al. 1995)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
\[ \log (P_t/kPa) = 7.32632 - 2550.1/(–28.65 + T/K), \text{ temp range 383–508 K, (Antoine eq., Stephenson & Malanowski 1987)} \]  
Henry’s Law Constant (Pa m³/mol at 25°C):  
Octanol/Water Partition Coefficient, log KOW:  
  2.1  (HPLC-RT correlation, McLeese et al. 1979)  
Octanol/Air Partition Coefficient, log KOA:  
Bioconcentration Factor, log BCF or log KB:  
Sorption Partition Coefficient, log KOC:  
Environmental Fate Rate Constants, k, and Half-Lives, t½:  
Half-Lives in the Environment:
14.1.1.17 *p*-tert-Butylphenol

![Chemical Structure](https://example.com/structure.png)

**Common Name:** 4-*tert*-Butylphenol  
**Synonym:** *p*-*tert*-butylphenol, 4-(α,α-dimethylethylphenol)  
**Chemical Name:** 4-*tert*-butylphenol, *p*-*tert*-butylphenol  
**CAS Registry No:** 98-54-4  
**Molecular Formula:** C_{10}H_{14}O, (CH_{3})_{3}CC_{6}H_{4}OH  
**Molecular Weight:** 150.217  
**Melting Point (°C):**  
98 (Lide 2003)  
**Boiling Point (°C):**  
237 (Lide 2003)  
**Density (g/cm³ at 20°C):**  
152.0 (20°C, Stephenson & Malanowski 1987)  
192.2 (calculated-Le Bas method at normal boiling point)  
**Acid Dissociation Constant, pKₐ:**  
9.90 (McLeese et al. 1979)  
**Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):**  
67.33, 50.62 (25°C, bp, Dreisbach 1955)  
50.54 (at normal boiling point, Handley et al. 1964)  
**Enthalpy of Fusion, ∆H₉₅ (kJ/mol):**  
**Entropy of Fusion, ∆S₉₅ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ∆S₉₅ = 56 J/mol K), F:** 0.192 (mp at 98°C)  
**Water Solubility (g/m³ or mg/L at 25°C or as indicated):**  
1000 (Thomas 1982)  
700 (Verschuereen 1983)  
580 (Yalkowsky et al. 1987)  
580 (shake flask-UV, Ahel & Giger 1993a)  
1850 (shake flask-HPLC/UV at pH 6.05, Varhančíková et al. 1995)  
753 (calculated-group contribution, 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):**  
6.402* (extrapolated-regression of tabulated data, temp range 70–238°C, Stull 1947)  
3.688 (extrapolated-Antoine eq., Dreisbach 1955)  
log (P/mmHg) = 7.49264 − 1999.8/(194.0 + t°C), temp range 140–370°C (Antoine eq. for liquid state, Dreisbach 1955)  
1.225* (liquid, extrapolated-Antoine eq., ebulliometry, measured range 198–251°C, Handley et al. 1964)  
log (P/mmHg) = 11.5638 − 3586.36/(t°C + 273); temp range 198–251°C (Antoine eq. from ebulliometric measurements, Handley et al. 1964)  
log (P/mmHg) = [–0.2185 × 13787.7/(T/K)] + 8.785696; temp range 70–238°C (Antoine eq., West 1972–73)  
5.072 (extrapolated-Cox eq., Chao et al. 1983)  
log (P/mmHg) = [1− 512.693/(T/K)] × 10^4{0.834403 − 2.10918 × 10⁻²·(T/K) + 0.554077 × 10⁻⁴·(T/K)²}; temp range 343.15–524.76 K (Cox eq., Chao et al. 1983)  
1.24 (supercooled liquid P₉₅, extrapolated-Antoine eq., Boublík et al. 1984)
log \( \frac{P}{kPa} = 6.12365 - 1626.256/(155.092 + t/°C) \); temp range 198–231.6°C (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublík et al. 1984)

1.25 (extrapolated-Antoine eq., Dean 1985)

log \( \frac{P}{mmHg} = 7.00038 - 1627.51/(155.24 + t/°C) \); temp range 198–252°C (Antoine eq., Dean 1985, 1992)

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

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

log \( \frac{P}{kPa} = 11.46945 - 4405.873/(T/K) \); temp range 280–304 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} = 6.13162 - 1632.939/(–117.258 + T/K) \), temp range: 471–525 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log \( \frac{P}{Pa} = 122.26679 – 8003.926/(T/K) – 40.16380\cdot\log (T/K) + 1.40155 \times 10^{-2}\cdot(T/K) \); temp range 471–525 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

log \( \frac{P}{mmHg} = –54.7404 – 2.4727 \times 10^{3}/(T/K) + 28.991\cdot\log (T/K) – 3.9356 \times 10^{-3}\cdot(T/K) + 1.543 \times 10^{-5}\cdot(T/K)^2 \); temp range 372–734 K (vapor pressure eq., Yaws 1994)

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

0.113 (calculated-\(1/K_{AW}\), \(C_w/C_A\) reported as exptl., Hine & Mookerjee 1975)

0.139; 3.750 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

0.922 (calculated-P/C, Thomas 1982)

0.113, 0.375 (quoted, calculated-MCI \(\chi\), Nirmalakhandan & Speece 1988)

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

3.04 (shake flask, Geyer et al. 1984)


3.41 (HPLC-RT correlation, Butte et al. 1987)

3.04 (recommended, Sangster 1989)

3.31 (recommended, Hansch et al. 1995)

3.10 (HPLC-RT correlation, Makovskaya et al. 1995b)

2.95 (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, log \(BCF\):

1.53 (Chlorella, after exposure to 50 µg/L for 24 h, Geyer et al. 1981)

1.88 (calculated-S, Geyer et al. 1981)

1.53; 2.08 (algae, golden orfe, Freitag et al. 1982)

2.38 (activated sludge, Freitag et al. 1982, 1985)

1.53 (Alga Chlorella fusca, wet weight basis, Geyer et al. 1984)

1.48; 2.07 (algae; golden ide, Freitag et al. 1985)

1.86 (zebrafish, Butte et al. 1987; quoted, Devillers et al. 1996)

2.38; 1.48; 2.07 (activated sludge; algae; fish; Freitag et al. 1987)

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

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

Volutilization: volatilization

\(t_{1/2} = 117\) h from water body with depth of 1 m (Thomas 1982).

Half-Lives in the Environment:
TABLE 14.1.1.17.1
Reported vapor pressures of \( p \)-tert-butylphenyl at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947

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<thead>
<tr>
<th>( t/°C )</th>
<th>P/Pa</th>
<th>( t/°C )</th>
<th>P/mmHg</th>
<th>( t/°C )</th>
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<td>114</td>
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<td>209.901</td>
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<td>eq. 2 P/mmHg</td>
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<td>191.5</td>
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<tr>
<td>214</td>
<td>53329</td>
<td>233.457</td>
<td>86724</td>
<td>( \Delta H_v/(kJ \cdot mol^{-1}) )</td>
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<td>238</td>
<td>101325</td>
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<td>92123</td>
<td>at bp    50.54</td>
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<td>m.p/°C 99.0</td>
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<td>251.608</td>
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Handley et al. 1964

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FIGURE 14.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for \( p \)-tert-butylphenol.
14.1.1.18 4-Octylphenol

Common Name: 4-Octylphenol
Synonym: \( p \)-octylphenol
Chemical Name: 4-octylphenol
CAS Registry No: 27193-28-8
Molecular Formula: \( \text{C}_{14}\text{H}_{22}\text{O} \)
Molecular Weight: 206.324
Melting Point (°C):
\[ 43 \] (Lide 2003)
Boiling Point (°C):
\[ 280-283 \] (Lewis 1996)
Density (g/cm³ at 20°C):
\[ 0.941 \] (at 24°C, Lewis 1996)
Molar Volume (cm³/mol):
\[ 281.0 \] (calculated-Le Bas method at normal boiling point)
Acid 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: 0.666 (mp at 43°C)
Water Solubility (g/m³ or mg/L at 25°C):
\[ 12.6 \pm 0.50 \] (generator column-HPLC/fluo., Ahel & Giger 1993a)
\[ 14.1 \pm 0.60 \] (shake flask-HPLC/UV, Varhaníčková et al. 1995)
Vapor Pressure (Pa at 25°C):
\[ 0.071 \] (quoted, Shiu et al. 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
\[ 0.4916 \] (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
\[ 3.70 \] (calculated-\( \pi \) substituent const. or fragment const., McLeese et al. 1981)
\[ 4.12 \pm 0.10 \] (shake flask-HPLC/fluo., Ahel & Giger 1993b)
Bioconcentration Factor, \( \log BCF \):
Sorption Partition Coefficient, \( \log K_{\text{OC}} \):
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):
Volutilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: average expctl. rate constant \( k = 0.0894 \text{ h}^{-1} \) compared to group contribution method predicted rate constants \( k = 0.1124 \text{ h}^{-1} \) (nonlinear) and \( k = 0.0982 \text{ h}^{-1} \) (Tabak & Govind 1993).
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
Half-Lives in the Environment:
14.1.1.19 4-Nonylphenol

Common Name: 4-Nonylphenol
Synonym: p-nonylphenol
Chemical Name: 4-nonylphenol
CAS Registry No: 104-40-5; 25154-52-3
Molecular Formula: C₁₅H₂₄O, C₉H₁₉C₆H₄OH
Molecular Weight: 220.351
Melting Point (°C): 42 (Lide 2003)
Boiling Point (°C): approx. 295 (Lide 2003)
Density (g/cm³ at 20°C): 1.513 (Budavari 1989)
Molar Volume (cm³/mol):
  231.1 (20°C, Stephenson & Malanowski 1987)
  303.2 (calculated-Le Bas method at normal boiling)
Acid Dissociation Constant, pKₐ:
Enthalpy of Fusion, ΔHₖₐₖ (kJ/mol):
Entropy of Fusion, ΔSₖₐₖ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₖₐₖ = 56 J/mol K), F: 0.681 (mp at 42°C)
Water Solubility (g/m³ or mg/L at 25°C):
  5.43 ± 0.17 (generator column-HPLC/fluo., Ahel & Giger 1993a)
  4.90 ± 0.4 (shake flask-GC/FID, Brix et al. 2001)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.0701* (ebulliometry, extrapolated, measured range 214.78–321.91°C, Hon et al. 1976)
  log (P/mmHg) = 7.74950 – 2550.67/(260.28 + t/°C); temp range 214.78–321.91°C (Antoine eq., ebulliometry, Hon et al. 1976)
  0.0720 (extrapolated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 6.8847 – 2560.53/(207.199 + t/°C), temp range 214.8–321.8°C (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)
  0.0691 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  0.174, 0.14, 0.109, 0.0908, 0.0802, 0.0556 (GC-RT correlation, 7 isomers, Bidleman & Renberg 1985)
Henry’s Law Constant (Pa m³/mol at 25°C):
  1.5705 (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, log Kₐₜₗₖ:
  4.20 (calculated-π substituent const. or fragment const., McLeese et al. 1981)
  4.10 (Geyer et al. 1982)
  5.90 (selected, Yoshida et al. 1986)
  5.76 (HPLC-RT correlation, Itoh et al. 1989)
  4.48 ± 0.12 (shake flask-HPLC/fluo., Ahel & Giger 1993b)
  6.36 (calculated-CLOGP 3.51, Jaworska & Schultz 1993)
6.36 (COMPUTOX, Kaiser 1993)
5.76 (Sangster 1993; Hansch et al. 1995)

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

Bioconcentration Factor, log $BCF$:
2.45 (salmon, McLeese et al. 1981)
1.00 (mussel *Mytilus edulis*, Geyer et al. 1982)
2.40 (fish liver, Ahel & Giger 1993a)
2.22; 2.45 (laboratory BCF data: killifish; salmon; Tsuda et al. 2000)
1.49; 1.32; 1.40; 1.34; 1.32; 1.18; 1.11–2.61 (field BCF data: pale chub; Ayu sweetfish, dark chub, crucian carp; large-mouth bass; bluegill; fish tissue; Tsuda et al. 2000)

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

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: average expl. rate constant of 0.0894 h$^{-1}$ compared to group contribution method predicted rate constants of 0.1124 h$^{-1}$ (nonlinear) and 0.0982 h$^{-1}$ (linear) (Tabak & Govind 1993).
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 45.0$ d$^{-1}$ (McLeese et al. 1981)
$k_2 = 0.16$ d$^{-1}$ (McLeese et al. 1981)

Half-Lives in the Environment:
Biota: $t_{1/2} = 4$ d in salmon before excretion (McLeese et al. 1981).

### TABLE 14.1.19.1
Reported vapor pressures of 4-nonylphenol at various temperatures

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<th>Hon et al. 1976</th>
<th>Ebuliometry</th>
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<td>$P/Pa$</td>
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log \( \log P = A - \frac{B}{(C + t/°C)} \)

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<td>C</td>
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\( \Delta H_v/(kJ \text{ mol}^{-1}) \)

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14.1.1.20 1-Naphthol

Common Name: 1-Naphthol
Synonym: α-naphthol, 1-naphthalenol, 1-hydroxynaphthalene
Chemical Name: 1-naphthol
CAS Registry No: 90-15-3
Molecular Formula: C_{10}H_{8}O, C_{10}H_{7}OH
Molecular Weight: 144.170
Melting Point (°C):
95
(Lide 2003)
Boiling Point (°C):
288.0 (sublimation, Weast 1982–83; Dean 1985; Lide 2003)
Density (g/cm³):
1.0989 (99°C, Weast 1982–83)
1.0954 (99°C, Dean 1985)
Acid Dissociation Constant, pKₐ:
9.20 (McLeese et al. 1979)
9.30 (Dean 1985)
Molar Volume (cm³/mol):
131.2 (99°C, Stephenson & Malanowski 1987)
155.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₜₚₑₜ (kJ/mol):
23.47 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔSₜₚₑₜ (J/mol K):
63.6 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔSₜₚₑₜ = 56 J/mol·K), F: 0.206 (mp at 95°C)
Water Solubility (g/m³ or mg/L at 25°C):
438 (quoted, Tsonopoulos & Prausnitz 1971)
870; 674 (exptl., calculated-group contribution, 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):
1.550* (extrapolated-regression of tabulated data, temp range 94–282.5°C, Stull 1947)
1333* (141.5°C, ebulliometry, measured range 141.5–282.5°C, Vontterres et al. 1955)
log (P/mmHg) = [–0.2185 × 14205.6/(T/K)] + 8.476669; temp range 94–282.5°C (Antoine eq., Weast 1972–73)
0.509 (extrapolated-liquid, Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.69308 – 2275.566/(202.869 + t/°C), temp range 141.5–282.5°C (Antoine eq. from reported exptl. data of Vontterres et al. 1955, Boublik et al. 1984)
0.290 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.28421 – 2077.56/(184.0 + t/°C); temp range 141–282°C (Antoine eq., Dean 1985, 1992)
log (Pₚ/kPa) = 12.20753 – 4873.394/(T/K); temp range 298–312 K (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)
log (Pₚ/kPa) = 10.70115 – 4405.522/(T/K); temp range 314–324 K (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)
log (Pₚ/kPa) = 7.53825 – 3083.8/(1.731 + T/K); temp range 399–556 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.49 (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log $K_{ow}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source and Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.98</td>
<td>(shake flask-UV, Hansch &amp; Anderson 1967)</td>
</tr>
<tr>
<td>2.98, 2.84, 2.31</td>
<td>(Hansch &amp; Leo 1979)</td>
</tr>
<tr>
<td>2.28</td>
<td>(HPLC-k′ correlation, Haky &amp; Young 1984)</td>
</tr>
<tr>
<td>2.84</td>
<td>(recommended, Sangster 1989, 1993)</td>
</tr>
<tr>
<td>2.84</td>
<td>(CPC centrifugal partition chromatography, Gluck &amp; Martin 1990)</td>
</tr>
<tr>
<td>3.13</td>
<td>(back-flushing-CPC centrifugal partition chromatography, Menges et al. 1990)</td>
</tr>
<tr>
<td>2.81</td>
<td>(shake flask-HPLC, Menges et al. 1991)</td>
</tr>
<tr>
<td>3.02</td>
<td>(concurrent chromatography, Berthod et al. 1988)</td>
</tr>
<tr>
<td>2.84</td>
<td>(COMPUTOX, Kaiser 1993)</td>
</tr>
<tr>
<td>2.43</td>
<td>(HPLC-RT correlation, Ritter et al. 1994)</td>
</tr>
<tr>
<td>2.84</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.64</td>
</tr>
<tr>
<td>3.33</td>
</tr>
<tr>
<td>3.41</td>
</tr>
<tr>
<td>2.10–2.77</td>
</tr>
<tr>
<td>2.63–2.99</td>
</tr>
<tr>
<td>1.84–2.1</td>
</tr>
<tr>
<td>1.99–2.66</td>
</tr>
<tr>
<td>1.30–1.90</td>
</tr>
<tr>
<td>2.89</td>
</tr>
<tr>
<td>2.52–2.96, 2.53</td>
</tr>
<tr>
<td>1.92–2.64</td>
</tr>
<tr>
<td>3.31, 2.91, 2.61</td>
</tr>
<tr>
<td>2.61; 3.48</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k and Half-Lives, $t_\text{½}$:

- **Volatilization:**
- **Photolysis:**
- **Photooxidation:**
- **Hydrolysis:**
- **Biodegradation:** average rate of biodegradation 38.4 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).
- **Biotransformation:**
- **Bioconcentration Uptake** ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environmental Compartments:
### TABLE 14.1.1.20.1
Reported vapor pressures of 1-naphthol at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>94.0</td>
<td>1333</td>
<td>141.5</td>
<td>1333</td>
</tr>
<tr>
<td>125.5</td>
<td>666.6</td>
<td>164.8</td>
<td>3333</td>
</tr>
<tr>
<td>142</td>
<td>1333</td>
<td>184.2</td>
<td>6666</td>
</tr>
<tr>
<td>158</td>
<td>2666</td>
<td>196.9</td>
<td>9999</td>
</tr>
<tr>
<td>177.8</td>
<td>5333</td>
<td>206.0</td>
<td>13332</td>
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<tr>
<td>190</td>
<td>7999</td>
<td>219.3</td>
<td>19998</td>
</tr>
<tr>
<td>206</td>
<td>13332</td>
<td>229.0</td>
<td>26664</td>
</tr>
<tr>
<td>229.6</td>
<td>26664</td>
<td>236.4</td>
<td>33330</td>
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<tr>
<td>255.8</td>
<td>53329</td>
<td>244.0</td>
<td>39997</td>
</tr>
<tr>
<td>282.5</td>
<td>101325</td>
<td>246.5</td>
<td>43330</td>
</tr>
<tr>
<td></td>
<td></td>
<td>250.2</td>
<td>46663</td>
</tr>
<tr>
<td></td>
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<td>255.1</td>
<td>53329</td>
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<td></td>
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<td>260.3</td>
<td>59995</td>
</tr>
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<td></td>
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<td>66661</td>
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<td></td>
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<td>265.7</td>
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<td>272.0</td>
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<td>275.2</td>
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<td>278.3</td>
<td>93325</td>
</tr>
<tr>
<td></td>
<td></td>
<td>282.5</td>
<td>101325</td>
</tr>
</tbody>
</table>

**mp/°C** 96.0

**b.p. = 288 °C**

**m.p. = 95 °C**

**FIGURE 14.1.1.20.1** Logarithm of vapor pressure versus reciprocal temperature for 1-naphthol.
14.1.1.21 2-Naphthol

Common Name: 2-Naphthol
Synonym: β-naphthol, 2-naphthalenol, 2-hydroxynaphthalene
Chemical Name: 2-naphthol
CAS Registry No: 135-19-3
Molecular Formula: C_{10}H_{7}OH
Molecular Weight: 144.170

Melting Point (°C):
121.5 (Lide 2003)

Boiling Point (°C):
285 (Lide 2003)

Density (g/cm³ at 20°C):
1.280 (Weast 1982–83)

Acid Dissociation Constant, pKₐ:
9.57 (Dean 1985)

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.79 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} (J/mol K):
47.7 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.113 (mp at 121.5°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):
680* (23.20°C, shake flask, measured range 15.55–31.25, McCune & Wilhelm 1949)
700 (20–25°C, Seidell 1941; Lange 1973)
713* (21.5°C, shake flask-UN spectrophotometry, measured range 6.9–75°C, Moyle & Tyner 1953)
754 (Tsonopoulos & Prausnitz 1971)
1000 (shake flask-UV spectrophotometry, Roberts et al. 1977)
740 (Verschueren 1983)
477 (calculated-group contribution, 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):
1.430* (extrapolated-regression of tabulated data, temp range 128.5–288°C, Stull 1947)
1333* (144.0°C, ebulliometry, measured range 144.0–288.0°C, Vontteres et al. 1955)

log (P/mmHg) = [–0.2185 × 14138.5/(T/K)] + 8.391271; temp range 128.6–288°C (Antoine eq., Weast 1972–73)
0.386 (extrapolated-Antoine eq., supercooled liquid P_L, Boublik et al. 1984)
log (P/kPa) = 6.62476 – 2244.555/(198.594 + t°C), temp range 144–288°C (Antoine eq. from reported exptl. data of Vontteres et al. 1955, Boublik et al. 1984)
0.160 (extrapolated-Antoine eq., supercooled liquid P_L, Dean 1985)

log (P/mmHg) = 7.34714 – 2135.0/(183.0 + t°C), temp range 144–288°C (Antoine eq., Dean 1985, 1992)
0.0303 (interpolated-Antoine eq.-III, solid P_S, Stephenson & Malanowski 1987)

log (P_L/kPa) = 12.48704 – 5110.333/(T/K), temp range 298–312 K (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 10.80636 – 4586.029/(T/K), temp range 314–332 K (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)

log (P_{II}/kPa) = 9.273 – 4112/(T/K), temp range 283–323 K (Antoine eq.-III, solid, Stephenson & Malanowski 1987)

log (P_{II}/kPa) = 7.22927 – 2827.5/(–19.868 + T/K), temp range 401–561 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
Phenolic Compounds

Henry’s Law Constant (Pa m³/mol at 25°C):
0.280 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
\[ \begin{align*}
&2.84 \quad \text{(shake flask-UV, Hansch & Anderson 1967)} \\
&2.70, 2.84, 2.89 \quad \text{(Hansch & Leo 1979)} \\
&2.01, 2.46 \quad \text{(HPLC-k' correlation, Eadsforth 1986)} \\
&2.84 \quad \text{(recommended, Sangster 1989)} \\
&2.85 \quad \text{(centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)} \\
&2.70 \quad \text{(EPA CLOGP Data Base, Hulzebos et al. 1993)} \\
&2.70 \quad \text{(COMPUTOX, Kaiser 1993)} \\
&2.70 \quad \text{(recommended, Hansch et al. 1995)}
\end{align*} \]

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \):
\[ \begin{align*}
&3.33 \quad \text{(soil, Means et al. 1982)} \\
&3.41 \quad \text{(soil, calculated-MCI \( \chi \), Sabljic 1987)} \\
&2.10–2.77 \quad \text{(soil, calculated-\( K_{ow} \) based on model of Karickhoff et al. 1979, Sabljic 1987)} \\
&2.63–2.99 \quad \text{(soil, calculated-\( K_{ow} \) based on model of Kenaga & Goring 1980, Sabljic 1987)} \\
&1.84–2.19 \quad \text{(soil, calculated-\( K_{ow} \) based on model of Briggs 1981, Sabljic 1987)} \\
&1.99–2.66 \quad \text{(soil, calculated-\( K_{ow} \) based on model of Means et al. 1982, Sabljic 1987)} \\
&1.30–1.90 \quad \text{(soil, calculated-\( K_{ow} \) based on model of Chiou et al. 1983, Sabljic 1987)}
\end{align*} \]

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

Volutilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 39.2 mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:
### TABLE 14.1.1.21.1
Reported aqueous solubilities and vapor pressures of 2-naphthol at various temperatures

<table>
<thead>
<tr>
<th>McCune &amp; Wilhelm 1949</th>
<th>Moyle &amp; Tyner 1953</th>
<th>Stull 1947</th>
<th>Vonterres et al. 1955</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aqueous solubility</strong></td>
<td><strong>Vapor pressure</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>shake flask</strong></td>
<td><strong>shake flask-UV spec.</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>ebulliometry</strong></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$S/g\cdot m^{-3}$</td>
<td>$t/°C$</td>
<td>$S/g\cdot m^{-3}$</td>
</tr>
<tr>
<td>15.55</td>
<td>501</td>
<td>6.90</td>
<td>355</td>
</tr>
<tr>
<td>16.24</td>
<td>526</td>
<td>13.45</td>
<td>487</td>
</tr>
<tr>
<td>23.20</td>
<td>680</td>
<td>17.7</td>
<td>561</td>
</tr>
<tr>
<td>31.25</td>
<td>928</td>
<td>21.5</td>
<td>713</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\log (100\cdot C_W) = A - B/(T/K)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_W$ g/100 mL</td>
</tr>
<tr>
<td>33.3</td>
</tr>
<tr>
<td>44.5</td>
</tr>
<tr>
<td>55.2</td>
</tr>
<tr>
<td>68.1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$m/°C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>122.5</td>
</tr>
<tr>
<td>254.2</td>
</tr>
<tr>
<td>269.0</td>
</tr>
<tr>
<td>276.6</td>
</tr>
<tr>
<td>283.0</td>
</tr>
</tbody>
</table>

### FIGURE 14.1.1.21.1
Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-naphthol.
FIGURE 14.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for 2-naphthol.
14.1.1.22 2-Phenylphenol (2-Hydroxybiphenyl)

Common Name: 2-Phenylphenol
Synonym: o-phenylphenol, 2-hydroxybiphenyl, [1,1′-biphenyl]-2-ol
Chemical Name: 2-phenylphenol
CAS Registry No: 90-43-7
Molecular Formula: C₁₂H₁₀O, C₆H₅C₆H₄OH
Molecular Weight: 170.206
Melting Point (°C):
  57.5 (Weast 1982–83)
Boiling Point (°C):
  286 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
  1.213 (Dean 1985)
  1.200 (25°C, Verschueren 1983)
Molar Volume (cm³/mol):
  192.0 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
  9.55 (Dean 1985)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
Entropy of Fusion, ΔSₘₙ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F: 0.480 (mp at 57.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
  700 (Verschueren 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):
  133.3* (100°C, summary of literature data, temp range 100–275°C, Stull 1947)
  1333* (161.9 °C, ebulliometry, measured range 161.9–275.0°C, Vonterrers et al. 1955)
  log (P/mmHg) = [–0.2185 × 15397.8/(T/K)] + 9.015370; temp range 100–275°C (Antoine eq., Weast 1972–73)
  log (P/mmHg) = [1– 549.249/(T/K)] × 10^{0.889463 – 4.72320 × 10 –4·(T/K) + 5.27654 × 10–7·(T/K)^2}; temp range 373.15–548.15 K (Cox eq., Chao et al. 1983)
  2667, 13330 (163 °C, 206°C, Verschueren 1983)
  log (P/kPa) = 5.50723 – 1137.035/(T/K) + 28.672272, temp range 161.9–275°C (Antoine eq. from reported exptl. data of Vonterrers et al. 1955, Boublík et al. 1984)
  30.0 (interpolated-Antoine eq.-I, solid Pₛ, Stephenson & Malanowski 1987)
  log (Pₛ/kPa) = 10.8635 – 4326.754/(T/K), temp range 291–314 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
  log (Pₛ/kPa) = 4.1553 – 547.8/–298.55 + T/K), temp range 434–547 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒw:
  3.09 (Hansch & Leo 1979)
  3.09 (COMPUTOX, Kaiser 1993)
  3.06 (HPLC-RT correlation, Ritter et al. 1994)
  3.09 (recommended, Sangster 1993)
  3.06 (HPLC-RT correlation, Ritter et al. 1994)
  3.09 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Vaporizaiton:

Photolysis:

Oxidation: photooxidation t_{1/2} = 66–3840 h in water, based on reported reaction rate constants for OH and RO_{2} radicals to react with phenol class compounds (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

photooxidation t_{1/2} = 0.1–22 h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_{3} radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Hydrolysis:

Biodegradation: 100% degradation under aerobic and anaerobic conditions after 3 wk (504 h) at 22°C (Verschueren 1983);

t_{1/2}(aq. aerobic) = 24–168 h, based on a river die-away study in which a 50% degradation was observed over a one week period (Gonsior et al. 1984; quoted, Howard et al. 1991); t_{1/2}(aq. anaerobic) = 96–672 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} = 0.1–22 h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_{3} radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Surface water: photooxidation t_{1/2} = 66–3840 h in water, based on reported reaction rate constants for OH and RO_{2} radicals to react with phenol class compounds (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991); t_{1/2} = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: t_{1/2} = 48–336 h, based on estimated 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 14.1.1.22.1
Reported vapor pressures of 2-phenylphenol at various temperatures

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Vonterres et al. 1955</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>summary of literature data</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>100</td>
<td>133.3</td>
</tr>
<tr>
<td>131.6</td>
<td>666.6</td>
</tr>
<tr>
<td>146.2</td>
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<td>163.3</td>
<td>2666</td>
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<td>180.3</td>
<td>5333</td>
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<td>275.0</td>
<td>101325</td>
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</table>

(Continued)
### TABLE 14.1.1.22.1 (Continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
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<td>56.6</td>
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<tr>
<td>275.0</td>
<td>101325</td>
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<tr>
<td>278.004</td>
<td></td>
</tr>
</tbody>
</table>

2-Phenylphenol (2-hydroxybiphenyl): vapor pressure vs. 1/T

**FIGURE 14.1.1.22.1** Logarithm of vapor pressure versus reciprocal temperature for 2-phenylphenol.
14.1.1.23 4-Phenylphenol (4-Hydroxybiphenyl)

Common Name: 4-Phenylphenol
Synonym: p-phenylphenol, 4-hydroxybiphenyl, [1,1'-biphenyl]-4-ol
Chemical Name: 4-phenylphenol
CAS Registry No: 92-69-3
Molecular Formula: C₁₂H₁₀O, C₆H₅C₆H₄OH
Molecular Weight: 170.206
Melting Point (°C): 166 (Lide 2003)
Boiling Point (°C): 305–308 (sublimation, Weast 1982–83; Stephenson & Malanowski 1987) 305 (Lide 2003)
Density (g/cm³ at 20°C):

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

Acid Dissociation Constant, pKₐ:
9.55 (Dean 1985)

Enthalpy of Fusion, ΔH_f (kJ/mol):
Entropy of Fusion, ΔS_f (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.0414 (mp at 166°C)

Water Solubility (g/m³ or mg/L at 25°C):
9.79 (CESARS 1988)
56.4; 50.2 (quoted exptl.; calculated-group contribution, 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):

log (P/mmHg) = (–0.2185 × 16974.3/(T/K)) + 9.234838; temp range 176.2–308°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = (1– 580.171/(T/K)) × 10⁸(0.949514 − 5.554686 × 10⁻¹(T/K) + 5.61184 × 10⁻⁷(T/K)²); temp range: 450.15–581.15 K, (Cox eq., Chao et al. 1983)
0.0278 (liquid, extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.97182 – 3214.349/(231.575 + t°C), temp range 177–308°C (Antoine eq. from reported exptl. data of Vonterrès et al. 1955, Boublik et al. 1984)
0.0200 (extrapolated-Antoine eq., Dean 1985)
log (P/kPa) = 8.6575 – 3022.8/(216.1 + t°C); temp range:177–308°C (Antoine eq., Dean 1985, 1992)
0.00153 (extrapolated-Antoine eq., solid Pₛ, Stephenson & Malanowski 1987)
log (Pₛ/kPa) = 11.17513 – 5066.6004/(T/K); temp range 327–348 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 8.41978 – 3684.9/(–5.81 + T/K), temp range 450–581 K (Antoine eq.-II., liquid, Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, log K_{ow}:
3.20 (shake flask-UV, Norrington et al. 1975)
3.63 (HPLC-RV correlation, Garst 1984)
2.88 (centrifugal partition chromatography (CPC), Terada et al. 1987)
3.20 (COMPUTOX databank, Kaiser 1993)
3.31 (HPLC-RT correlation, Ritter et al. 1994)
3.20  (recommended, Sangster 1993)
3.20  (recommended, Hansch et al. 1995)
2.60, 2.56, 2.70, 2.72 (HPLC-k correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, log BCF:

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

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 14.1.1.23.1</th>
<th>Reported vapor pressures of 4-phenylphenol at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stull 1947 summary of literature data</td>
</tr>
<tr>
<td></td>
<td>t/°C</td>
</tr>
<tr>
<td>176.2</td>
<td>1333</td>
</tr>
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<td>193.8</td>
<td>2666</td>
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<td>213.0</td>
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<td>225.3</td>
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<td>240.9</td>
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<td>53329</td>
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<td>308.0</td>
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<tr>
<td>mp/°C</td>
<td>164.5</td>
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<td></td>
<td>Vonterres et al. 1955 ebulliometry</td>
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<tr>
<td></td>
<td>t/°C</td>
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<td>177.0</td>
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<td>199.2</td>
<td>3333</td>
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<td>217.8</td>
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<td>bp/°C</td>
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</table>
14.1.2 CHLOROPHENOLS

14.1.2.1 2-Chlorophenol

Common Name: 2-Chlorophenol
Synonym: \textit{o}-chlorophenol, 1-chloro-2-hydroxybenzene
Chemical Name: 2-chlorophenol
CAS Registry No: 95-57-8
Molecular Formula: C\textsubscript{6}H\textsubscript{4}(OH)Cl
Molecular Weight: 128.556
Melting Point (°C):
9.4 (Lide 2003)
Boiling Point (°C):
174.9 (Dreisbach 1955; Weast 1982–83; Lide 2003)
Density (g/cm\textsuperscript{3}):
1.2634 (20°C, Weast 1982–83)
1.257 (25°C, Krijgsheld & van der Gen 1986)
Acid Dissociation Constant, pK\textsubscript{a}:
8.65 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)
8.48 (Pearce & Simkins 1968; Krijgsheld & van der Gen 1986)
8.52 (Drahonovsky & Vacek 1971)
8.29 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)
8.55 (Serjeant & Dempsey 1979)
8.30 (Hoigné & Bader 1983)
9.30 (HPLC, Miyake et al. 1987)
Molar Volume (cm\textsuperscript{3}/mol):
101.8 (20°C, Stephenson & Malanowski 1987)
124.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \Delta H\textsubscript{v} (kJ/mol):
40.05, 49.25 (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, \Delta H\textsubscript{fus} (kJ/mol):
13.50 (Dreisbach 1955)
10.75 (Tsonopoulos & Prausnitz 1971)
12.52 (Chickos et al. 1999)
Entropy of Fusion, \Delta S\textsubscript{fus} (J/mol K):
38.12 (Tsonopoulos & Prausnitz 1971)
44.24 (exptl., Chickos et al. 1999)
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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
25000* (20°C, synthetic method, measured range –0.20 to 173.0°C, Sidgwick & Turner 1922)
29000 (20–25°C, Seidell 1941; Urano et al. 1982)
24650 (20°C, shake flask-UV, Mully & Metcalf 1966)
22000 (shake flask-spectrophotometry, Roberts et al. 1977)
28500 (20°C, Verschueren 1977, 1983)
11480 (shake flask-LSC, Banerjee et al. 1980)
11200 (shake flask-radioactive analysis, Veith et al. 1980)
20000 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)
23260 (shake flask-HPLC/UV at pH 4.8, Ma et al. 1993)
28500 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
22660* (24.6°C, shake flask-conductimetry, measured range 15.4–34.5°C, Achard et al. 1996)

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

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>316*</td>
<td>(interpolated-regression of tabulated data, temp range 12.7–174.5°C, Stull 1947)</td>
<td></td>
</tr>
<tr>
<td>208</td>
<td>(calculated-Antoine eq., Dreisbach 1955)</td>
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<tr>
<td>313</td>
<td>(extrapolated from Antoine eq., Weast 1972–73)</td>
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<tr>
<td>5532</td>
<td>(80°C, Verschueren 1977, 1983)</td>
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<tr>
<td>293, 180.7</td>
<td>(extrapolated, Antoine eq., Dean 1985)</td>
<td></td>
</tr>
<tr>
<td>313</td>
<td>(extrapolated from Antoine eq., Stephens &amp; Malanowski 1987)</td>
<td></td>
</tr>
<tr>
<td>131.8</td>
<td>(extrapolated-Antoine eq., Stephens &amp; Malanowski 1987)</td>
<td></td>
</tr>
<tr>
<td>737, 1329, 2278, 3736, 5907</td>
<td>(50, 60.24, 69.94, 79.95, 89.94°C, calculated-Antoine eq. of Stephens &amp; Malanowski 1987, Tabai et al. 1997)</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.065</td>
<td>(calculated-P/C, Mabey et al. 1982)</td>
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<tr>
<td>0.688</td>
<td>(calculated-P/C, Shiu et al. 1994)</td>
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<tr>
<td>0.661</td>
<td>(20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)</td>
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</table>

Octanol/Water Partition Coefficient, log K OW:

<table>
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<tr>
<th>Temperature</th>
<th>Method</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.15</td>
<td>(shake flask-UV, Fujita et al. 1964;)</td>
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<td>2.15, 2.19</td>
<td>(Leo et al. 1971)</td>
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<td>2.20</td>
<td>(calculated using data from Fujita et al. 1964, Umeyama et al. 1971)</td>
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<tr>
<td>2.12</td>
<td>(20°C, shake flask, Korenman 1974)</td>
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<tr>
<td>2.15</td>
<td>(LC-k‘ correlation, Carson et al. 1975)</td>
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<tr>
<td>2.17</td>
<td>(Hansch &amp; Leo 1979)</td>
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</tr>
<tr>
<td>2.16</td>
<td>(shake flask-LSC, Banerjee et al. 1980)</td>
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</tr>
<tr>
<td>0.83</td>
<td>(RP-HPLC-RT correlation, Veith et al. 1980)</td>
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<tr>
<td>2.11</td>
<td>(RP-HPLC-RT correlation, Butte et al. 1981)</td>
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<tr>
<td>2.03</td>
<td>(shake flask, Dearden &amp; Bresnen 1981)</td>
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<td>2.16 ± 0.03</td>
<td>(HPLC-k’ correlation, Hammers et al. 1982)</td>
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<tr>
<td>2.32</td>
<td>(RP-HPLC-RT correlation, Chin et al. 1986)</td>
<td></td>
</tr>
<tr>
<td>1.56, 1.99</td>
<td>(HPLC-k’ correlation, Eadsforth 1986)</td>
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<tr>
<td>2.09</td>
<td>(HPLC-RT correlation, Miyake et al. 1986)</td>
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</tr>
<tr>
<td>2.13</td>
<td>(shake flask-UV, Miyake et al. 1987)</td>
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<tr>
<td>2.16</td>
<td>(shake flask-CPC, Berthod et al. 1988)</td>
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<td>2.24</td>
<td>(batch equilibration-UV, Beltrame et al. 1988)</td>
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<tr>
<td>2.11</td>
<td>(centrifugal partition chromatography, Gluck &amp; Martin 1990)</td>
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<tr>
<td>2.25</td>
<td>(back flashing-CPC centrifugal partition chromatography; Menges et al. 1990)</td>
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<td>2.05</td>
<td>(centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)</td>
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<tr>
<td>2.17</td>
<td>(counter-current chromatography, Berthod et al. 1992)</td>
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</tr>
<tr>
<td>2.15</td>
<td>(recommended, Sangster 1993)</td>
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<tr>
<td>2.29</td>
<td>(shake flask-GC, Kishino &amp; Kobayashi 1994)</td>
<td></td>
</tr>
<tr>
<td>2.15</td>
<td>(recommended, Hansch et al. 1995)</td>
<td></td>
</tr>
</tbody>
</table>
Bioconcentration Factor, log BCF:

- 2.33 (bluegill sunfish, Barrows et al. 1980)
- 2.33 (bluegill sunfish, Veith et al. 1980)
- 1.61 (microorganisms-water, calculated-K\textsubscript{OW}, Mabey et al. 1982)
- 2.33 (bluegill sunfish, Bysshe 1982)
- 0.81 (gold fish, Kobayashi et al. 1979; quoted, Verschueren 1983; Howard 1989)
- 0.81 (Isnard & Lambert 1988)
- 0.28–1.40 (estimated from K\textsubscript{OW}, Howard 1989)

Sorption Partition Coefficient, log K\textsubscript{OC}:

- 3.70, 3.60 (sediment: fine, coarse; Isaacson & Frink 1984)
- 1.86 (sediment-water, calculated-K\textsubscript{OW}, Mabey et al. 1982)
- 1.71 (clay loam soil, Boyd 1982; quoted, Howard 1989)
- 3.69 (untreated fine sediment, Isaacson & Frink 1984)
- 3.60 (untreated coarse sediment, Isaacson & Frink 1984)
- 3.98 (treated fine sediment, Isaacson & Frink 1984)
- 4.36 (treated coarse sediment, Isaacson & Frink 1984)
- 1.20–2.55 (estimated from K\textsubscript{OW}, Howard 1989)
- 1.82 (calculated-K\textsubscript{OW}, Kollig 1993)
- 2.60 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

- Volatilization: \( t_{1/2} = 1.35, 1.60 \) h from stirred and static water at 23.8°C (Chiou et al. 1980; Howard 1989); \( t_{1/2} = 73 \) d, based on estimation from a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).
- Photolysis: vapor phase \( t_{1/2} = 47 \) h (Howard 1989); first-order photolysis disappearance rate constant \( k = 3.01 \times 10^{-2} \) min\(^{-1}\) in the absence of DOM at 313 nm (Kawaguchi 1992).
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \), with O\(_3\) or as indicated, \({ }^{\ast}\)data at other temperatures see reference: \( k_{\text{aq.}} \leq 7 \times 10^{-10} \text{M}^{-1} \text{h}^{-1}\) for singlet oxygen and \( 1 \times 10^{-7} \text{M}^{-1} \text{h}^{-1}\) for peroxy radical at 25°C (Mabey et al. 1982)

\( k_{\text{aq.}} = 66 \times 10^{-6} \text{M}^{-1} \text{s}^{-1}\) at pH 8, \( k = (1.1 \pm 0.3) \times 10^{3} \text{M}^{-1} \text{s}^{-1}\) for non-protonated species, \( k = (0.2 \pm 0.1) \times 10^{9} \text{M}^{-1} \text{s}^{-1}\) for phenolate ions for the reaction with ozone in water using 3 mM t-BuOH as scavenger at pH 1.8–4 and 20–23°C (Hoigné & Bader 1983b)

\( k_{\text{OH}} = 1.3 \times 10^{-11} \text{cm}^{3} \text{molecule}^{-1} \text{s}^{-1}\) for reaction with OH radical in air (Bunce et al. 1991)

\( k_{\text{aq.}} = (9.2 \pm 9.4) \times 10^{6} \text{M}^{-1} \text{h}^{-1}\) for the reaction with singlet oxygen in aqueous phosphate buffer at 27 ± 1°C (Tratnyek & Hoigné 1991)

Hydrolysis:

Biodegradation: average rate \( k = 25.0 \text{ mg COD g}^{-1} \text{ h}^{-1}\) based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); time necessary for complete degradation of 16 m/L in 14–25 d by wastewater (Haller 1978);

aerobic degradation in a non-sterile clay loam soil: 91% loss at 0°C after 8 d at the termination of the experiment, 94% loss at 4°C after 8 d and 100% loss at 20°C after 10–15 d all under same expltl. conditions (Baker et al. 1980);

rate constants \( k = 1.0 \text{ d}^{-1}\) with \( t_{1/2} = 0.7 \text{ d}\) in adopted activated sludge and \( k = 0.3 \text{ d}^{-1}\) with \( t_{1/2} = 2.3 \text{ d}\) in soil suspension under aerobic conditions (Mills et al. 1982); completely degraded in soil suspensions in 14 d and by a soil microflora within 64 d (quoted, Verschueren 1983);

approximately 48 h in a column microcosm under aerobic conditions (Suflita & Miller 1985); degradation rate \( k = 10 \text{ -mol L}^{-1} \text{ d}^{-1}\) in freshwater and \( k = 8 \text{ -mol L}^{-1} \text{ d}^{-1}\) in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990).

Biotransformation: rate constant for bacterial transformation of \( 1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}\) in water (Mabey et al. 1982); microbial transformation \( k = (7.1 \pm 1.6) \times 10^{-11} \text{ L organism}^{-1} \text{ h}^{-1}\) (Paris et al. 1983; quoted, Steen 1991); degradation \( k = 3.49 \times 10^{-17} \text{ (± 38% SD) mol cell}^{-1} \text{ h}^{-1}\) from pure culture studies (Banerjee et al. 1984).

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

Air: half-life in the atmosphere was estimated to be 1.96 d (Howard 1989); tropospheric lifetime of 1 d, calculated based on reactions principally with OH radical on March 21 at 43°N (Bunce 1991).

Surface water: $t_{1/2} = 16.8$ d in sludge and $t_{1/2} = 55.2$ d in polluted river waters (Mills et al. 1982); rate constant of $(1.1 \pm 0.3) \times 10^3$ M$^{-1}$ s$^{-1}$ for the reaction with ozone at pH 1.8–4.0 (Hoigné & Bader 1983b); photolysis disappearance $k = 3.01 \times 10^{-2}$ min$^{-1}$ in the absence of DOM at 313 nm (Kawaguchi 1992).

Groundwater:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 14 d in Dunkirk silt loam, 47 d in Mardin silt loam (Alexander & Aleem 1961)

$\text{t}_{1/2} = 51$ d in a coarse sandy soil, $\text{t}_{1/2} = 110$ d in sandy loam (Kjeldsen et al. 1990)

$\text{t}_{1/2} = 7.2$ d in an acidic clay soil with < 1.0% organic matter and $\text{t}_{1/2} = 1.7$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota: $\text{t}_{1/2} < 1$ d in tissue of bluegill sunfish (Barrows et al. 1980).

---

**TABLE 14.1.2.1.1**

Reported aqueous solubilities and vapor pressures of 2-chlorophenol at various temperatures

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<tr>
<th></th>
<th>Aqueous solubility</th>
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<td></td>
<td>Sidgwick &amp; Turner</td>
<td>Achard et al. 1996</td>
<td>Stull 1947</td>
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<td>synthetic method</td>
<td>shake flask-conductimetry</td>
<td>summary of literature data</td>
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<td>S/g⋅m$^{-3}$</td>
<td>S/g⋅m$^{-3}$</td>
<td>t/$^\circ$C</td>
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<td>−0.20</td>
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<td>100000</td>
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</table>

Critical solution temp 173°C
**FIGURE 14.1.2.1.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-chlorophenol.

**FIGURE 14.1.2.1.2** Logarithm of vapor pressure versus reciprocal temperature for 2-chlorophenol.
14.1.2.2 3-Chlorophenol

Common Name: 3-Chlorophenol
Synonym: m-chlorophenol, 1-chloro-3-hydroxybenzene
Chemical Name: 3-chlorophenol
CAS Registry No: 108-43-0
Molecular Formula: C₆H₄ClOH
Molecular Weight: 128.556
Melting Point (°C):
32.6  (Lide 2003)
Boiling Point (°C):
214.0  (Sidgwick & Turner 1922; Stull 1947; Weast 1982–83; Lide 2003)
Density (g/cm³, 20°C):
1.268  (25°C, Weast 1982–83)
Acid Dissociation Constant, pKₐ:
9.12  (Farquharson et al. 1958; Renner 1990)
8.85  (Doedens 1967; Jones 1981; Bintein & Devillers 1994)
9.08  (Pearce & Simkins 1968)
8.78  (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)
9.10  (Dean 1985; Schultz & Cajina-Quezada 1987)
9.02  (Krijgsheld & van der Gen 1986)
Molar Volume (cm³/mol):
103.3  (45°C, Stephenson & Malanowski 1987)
124.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
11.72  (Tsonopoulos & Prausnitz 1971)
14.91; 15.6  (expnl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_fus (J/mol K):
38.2  (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol·K), F: 0.842 (mp at 9.4°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):
26000*  (20°C, synthetic method, measured range –0.20 to 130.8°C, Sidgwick & Turner 1922)
26000  (20–25°C, Seidell 1941; Urano et al. 1982; Shigeoka et al. 1988)
22420  (20°C, Mulley & Metcalf 1966)
22000  (recommended, Horvath & Getzen 1985)
22190  (shake flask-HPLC/UV at pH 4.6, Ma et al. 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):
41.90*  (extrapolated-regression of tabulated data, temp range 44.2–214°C, Stull 1947)
41.40  (extrapolated-Antoine eq., liquid value, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 11979.7/(T/K)] + 8.276287; temp range 44.2–214°C (Antoine eq., Weast 1972–73)
667.0  (72°C, Verschueren 1983)
1.034  (extrapolated-Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log \( (P_s/kPa) = 7.61412 – 3178.132/(T/K) \), temp range 252–293 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

33.40  (extrapolated-Antoine eq., supercooled liquid \( P_L \), Stephenson & Malanowski 1987)

\[ \log (P_L/kPa) = 6.54908 – 1978.86/(-51.572 + T/K) \], temp range 317–487 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol):

0.0567  (calculated, Hine & Mukerjee 1975)

0.2045  (calculated-P/C, Shiu et al. 1994)


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

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

2.55  (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)

2.52  (shake flask-UV, Korenman 1974)

2.17, 2.29  (calculated-\( \pi \) const., calculated-fragment const., Rekker 1977)

2.50  (Hansch & Leo 1979)

2.33  (HPLC-\( k' \) correlation, Butte et al. 1981, Butte et al. 1987)

2.44  (Dearden & Bresnen 1981)

2.36  (HPLC-\( k' \) correlation, Hammers et al. 1982)

2.55  (RP-HPLC-\( k' \) correlation, Miyake & Terada 1982)

1.87, 2.29  (HPLC-\( k' \) correlation, Eadsforth 1986)

2.36  (HPLC-RT correlation, Miyake et al. 1986)

2.55  (batch equilibration-UV, Beltrame et al. 1988)

2.50  (RP-HPLC-capacity ratio correlation, Minick et al. 1988)

2.48  (RP-HPLC, Shigeoka et al. 1988)

2.43; 2.63  (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.50  (recommended, Sangster 1993)

2.64  (shake flask-GC, Kishino & Kobayashi 1994)

2.50; 2.57  (HPLC-RT correlation, electrometric titration, Slater et al. 1994)

2.50  (recommended, Hansch et al. 1995)

2.60  (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, \( \log BCF \):

1.30  (Golden ide, Freitag et al. 1985)

1.25  (zebrafish, Butte et al. 1987)

0.845, 1.23  (earthworms \( e. fetaida andrei \): Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

2.01, 2.09  (earthworms \( l. rubellus \): Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

1.17–2.55  (estimated from \( K_{OW} \), Howard 1989)

1.00, 1.32, 2.17, 2.18  (earthworm system, from literature, Connell & Markwell 1990)

1.10, 1.40, 10.1, 16.3  (earthworm system, derived data, Connell & Markwell 1990)

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

1.20–2.74  (estimated from \( K_{OW} \), Howard 1989)

2.54  (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Volatilization: estimated \( t_{1/2} \approx 73 \) d for evaporation from a model river of 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: vapor phase \( t_{1/2} = 1.96 \) d (Howard 1989);

measured pseudo-first-order reaction \( k = 0.048 \pm 0.001 \) min\(^{-1}\) for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).
Oxidation: rate constant $k = (5.4 \pm 1.0) \times 10^6$ M$^{-1}$ s$^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at 27 ± 1°C (Tratnyek & Hoigné 1991).

Hydrolysis: will not be an important degradation process (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964); completely degraded in soil suspensions within 72 d and by a soil microflora within 64 d (quoted, Verschueren 1983); time necessary for complete degradation of 16 mg/L in 14–25 d by wastewater (Haller 1978); degradation rate of 15 -mol L$^{-1}$ d$^{-1}$ in freshwater and 18 µmol L$^{-1}$ d$^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990).

Biotransformation: degradation rate of 4.32 × 10$^{-17}$ (± 47% SD) mol cell$^{-1}$ h$^{-1}$ from pure culture studies (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air: vapor phase half-life was estimated to be 1.96 d (Howard 1989).

Surface water: $t_{1/2} = (14.5 \pm 0.3)$ min for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment: half-life was approximately 30 d in sediment from a farm stream at 20°C (Howard 1989).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961) disappearance $t_{1/2} = 2.5$ d from Kooyenburg soil, $t_{1/2} = 5.4$ d from Holten soil with earthworms *Eisenia fetida andrei* and $t_{1/2} = 2.6$ d from Kooyenburg soil, $t_{1/2} = 2.1$ d from Holten soil with earthworms *Eisenia fetida* andrewi (van Gestel & Ma 1988);

$15.1$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 21.8$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

### TABLE 14.1.2.2.1
Reported aqueous solubilities and vapor pressures of 3-chlorophenol at various temperatures

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<th>Temperature (°C)</th>
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<th>Vapor pressure (P/Pa)</th>
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<td>S/g·m$^{-3}$</td>
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**FIGURE 14.1.2.2.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-chlorophenol.

**FIGURE 14.1.2.2.2** Logarithm of vapor pressure versus reciprocal temperature for 3-chlorophenol.
14.1.2.3 4-Chlorophenol

Common Name: 4-chlorophenol
Synonym: p-chlorophenol, 1-chloro-4-hydroxybenzene
Chemical Name: 4-chlorophenol
CAS Registry No: 106-48-9
Molecular Formula: ClC₆H₄OH
Molecular Weight: 128.556
Melting Point (°C): 42.8 (Lide 2003)
Boiling Point (°C): 220 (Lide 2003)
Density (g/cm³ at 20°C): 1.2651 (Weast 1982–83)
Acid Dissociation Constant, pKₐ: 9.37 (Farquharson et al. 1958; Ugland et al. 1981; Saarikoski & Viluksela 1982; Renner 1990)
9.18 (Doedens 1967)
9.42 (Pearce & Simkins 1968)
9.41 (Serjeant & Dempsey 1979)
9.20 (Hoigné & Bader 1983)
9.43 (Dean 1985; Schultz & Cajina-Quezada 1987)
9.37 ± 0.01 (potentiometric partition, Hersey et al. 1989)
9.57 ± 0.01 (UV with pH profile, Hersey et al. 1989)
Molar Volume (cm³/mol):
101.6 (40°C, Stephenson & Malanowski 1987)
124.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₙₐₙ (kJ/mol):
14.69 (Tsonopoulos & Prausnitz 1971)
14.07; 16.2 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔSₙₐₙ (J/mol K):
46.44 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔSₙₐₙ = 56 J/mol K), F: 0.669 (mp at 42.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
27000* (20°C, synthetic method, measured range –0.20 to 128.7°C, Sidgwick & Turner 1922)
27000 (20–25°C, Seidell 1941; Urano et al. 1982)
27000 (shake flask-UV at pH 5.1, Blackman et al. 1955)
26250 (20°C, shake flask-UV, Mulley & Metcalf 1966)
24000 (shake flask-spectrophotometry, Roberts et al. 1977)
27000 (recommended, Horvath & Getzen 1985)
26390 (shake flask-HPLC/UV at pH 4.6, Ma et al. 1993)
25540* (25.2°C, shake flask-conductimetry, measured range 15.1–34.5°C, Achar et al. 1996)
20712* (11.05°C, shake flask-optical method, measured range 282.2–386.1 K, Jaoui et al. 1999)

\[ \ln \left[ \frac{S}{(\text{mol kg}^{-1})} \right] = 5.6451 - 716.81/(T/K) \]; temp range 282–342 K (eq. derived using reported exptl. data, Jaoui et al. 2002)
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):

28.6* (extrapolated-regression of tabulated data, temp range 49.8–220°C, Stull 1947)
28.0 (extrapolated-Antoine eq., liquid value, Weast 1972–73)

log (P/mmHg) = [–0.2185 × 12281.6/(T/K)] + 8.331937; temp range 49.8–220°C (Antoine eq., Weast 1972–73)

3.47 (extrapolated liquid value, Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 8.83238 – 1385.1/(–131.1 + T/K), temp range 373–493 K (Antoine eq., Stephenson & Malanowski 1987)

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

0.0567 (calculated, Hine & Mookerjee 1975; Howard 1989)
0.0471 (calculated-P/C, Leuenberger et al. 1985)
0.0952 (calculated-P/C, Shiu et al. 1994)

kH/kPa = 2017.07 – 110385.0/(T/K) – 290.078; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, log K OW:

2.39 (shake flask-UV, Fujita et al. 1964)
2.53 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
2.37 (HPLC-RT correlation, Carlson et al. 1975)
2.40 (HPLC-RT correlation, Mirreles et al. 1976)
2.17, 2.29 (calculated-π const., calculated-fragment const., Rekker 1977)
2.35, 2.39, 2.44, 2.40 (lit. values, Hansch & Leo 1979)
2.51 (calculated-π const. or fragment const., McLeese et al. 1979)
2.55 (20°C, shake flask-UV, Rogers & Wong 1980)
2.35 (HPLC-k’ correlation, Hammers et al. 1982)
2.51 (RP-HPLC-k’, correlation Miyake & Terada 1982)
2.46 ± 0.06 (HPLC-RV correlation.-ALPM, Garst & Wilson 1984)
2.88 (CPC-RV, Terada et al. 1987)
2.43 (batch equilibration-UV, Beltrame et al. 1988, Beltrame et al. 1989)
2.39 (RP-HPLC-capacity ratio, Minick et al. 1988)
2.41 (shake flask, Shigeoka et al. 1988)
2.42; 2.46; 2.34, 2.45 (filter chamber-UV; potentiometric partition; Hersey et al. 1989)
2.52; 2.59 (shake flask; HPLC-RT correlation, Wang et al. 1989)
2.39 (recommended, Sangster 1993)
2.63 (shake flask-GC, Kishino & Kobayashi 1994)
2.41; 2.45 (HPLC-RT correlation, electometric titration, Slater et al. 1994)
2.39 (recommended, Hansch et al. 1995)
1.82, 1.83, 2.01, 1.98 (HPLC-k’ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, log BCF:

1.18 (goldfish, Kobayashi et al. 1979)
0.30–1.59 (estimated from K OW, Howard 1989)
1.05–1.50 (estimated, NCASI 1992)

Sorption Partition Coefficient, log K OC:

1.85 (clay loam soil, Boyd 1982; Howard 1989)
1.20–2.68 (estimated from K OW, Howard 1989)
2.142, 1.966, 1.966, 2.289, 1.952 (soils, 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)
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

**Vaporization:** half-lives of 12.8 h, 17.4 h for evaporation from stirred and static water at a depth of 0.38 cm at 23.6°C (Chiou et al. 1980; Howard 1989); \( t_{1/2} = 73 \) d was estimated for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).

**Photolysis:**
- photo-transformation rate constants: \( k = 0.011 \) h\(^{-1}\) with \( t_{1/2} = 63 \) h for distilled water in summer (mean temp 25°C) and \( k = 0.007 \) h\(^{-1}\) with \( t_{1/2} = 99 \) h in winter (mean temp 14°C); \( k = 0.03 \) h\(^{-1}\) with \( t_{1/2} = 28 \) h for estuarine water in summer and \( k = 0.011 \) h\(^{-1}\) with \( t_{1/2} = 63 \) h in winter exposed to full sunlight and microbes (Hwang et al. 1986).
- photo-mineralization rate constants: \( k = 0.012 \) h\(^{-1}\) with \( t_{1/2} = 58 \) d for distilled water in summer and \( k = 0.003 \) h\(^{-1}\) with \( t_{1/2} = 224 \) d in winter; \( k = 0.07 \) h\(^{-1}\) with \( t_{1/2} = 10 \) d in summer and \( k = 0.007 \) h\(^{-1}\) with \( t_{1/2} = 95 \) d in winter for surface estuarine water exposed to full sunlight and microbes (Hwang et al. 1986);
- photo-degradation \( k = 564 \times 10^3 \) min\(^{-1}\) with \( t_{1/2} = 1.1 \) min for direct UV radiation in aqueous solutions (Benitez et al. 2000).

**Oxidation:** rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with \( \text{NO}_3 \) radical and \( k_{\text{O}_3} \) with \( \text{O}_3 \) or as indicated, *data at other temperatures see reference:*
- \( k_{\text{aq.}} = (600 \pm 100) \) M\(^{-1}\)s\(^{-1}\) for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983a).
- \( k_{\text{aq.}} = 34 \times 10^6 \) M\(^{-1}\)s\(^{-1}\) at pH 8, and \( k = (600 \pm 100) \) M\(^{-1}\)s\(^{-1}\) for non-protonated species, \( k = (0.6 \pm 0.2) \times 10^6 \) M\(^{-1}\)s\(^{-1}\) for phenolate ions for the reaction with ozone in water using 3 mM t-BuOH as scavenger at pH 1.5–6 and 20–23°C (Hoigné & Bader 1983b).
- \( k_{\text{aq.}} = (6.0 \pm 3.6) \times 10^6 \) M\(^{-1}\)s\(^{-1}\) for the reaction with singlet oxygen in aqueous buffer at 27 ± 1°C (Tratnyek & Hoigné 1991).
- 72.1 mg/L total organic carbon (TOC) degraded to 98% TOC after 5 h illumination with 250 watt tungsten lamp by the photo-Fenton reaction (Ruppert et al. 1993).
- \( k = 1877 \times 10^3 \) min\(^{-1}\) with a half-life of 0.4 min for reaction with Fenton’s reagent; \( k_{\text{O}_3} = 17 \times 10^3 \) min\(^{-1}\) with a half-life of 38.15 min at pH 2; and \( k_{\text{O}_3} = 239 \times 10^3 \) min\(^{-1}\) with a half-life of 3.4 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

**Hydrolysis:**

**Biodegradation:** 95% degradation in 3–6 d in a mixed bacteria cultures (Tabak et al. 1964);
- average rate of biodegradation 11.0 mg COD g\(^{-1}\) h\(^{-1}\) based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
- time necessary for complete degradation of 16 mg/L in 7–14 d by wastewater and in 14–25 d by soil (Haller 1978);
- \( t_{1/2} = 475 \) h in river waters with a calculated first-order \( k = 0.035 \) d\(^{-1}\) (Lee & Ryan 1979; quoted, Battersby 1990);
- aerobic degradation in a non-sterile clay-loam soil: 77% loss at 0°C at the termination of the experiment after 14 d, 84% loss at 4°C after 12 d and 100% loss at 20°C after 30 d all under same experimental conditions (Baker et al. 1980);
- \( t_{1/2} = 216–480 \) h and 72–1080 h for 75% degradation in mineral medium and seawater (de Kreuk & Hanstveit 1981);
- biodegradation first order rate constant \( k = 0.23 \) d\(^{-1}\) in aquatic systems (Scow 1982);
- completely degraded in soil suspensions in 9 d and by a soil microflora in 16 d (quoted, Verschueren 1983);
- microbial degradation is the primary transformation process; transformation \( k = 0.06 \) h\(^{-1}\) with \( t_{1/2} = 11 \) h for estuarine water in summer and \( t_{1/2} = 0.006 \) h\(^{-1}\) with \( t_{1/2} = 116 \) h in winter in the darkness (Hwang et al. 1986);
- mineralization \( k = 0.293 \) h\(^{-1}\) with \( t_{1/2} = 2 \) d for estuarine water in summer and \( k = 0.003 \) h\(^{-1}\) with \( t_{1/2} = 231 \) d in winter in the darkness (Hwang et al. 1986); degradation rate constants \( k = 0.035 \) d\(^{-1}\) with \( t_{1/2} = 480 \) d in Skidway River water and 0.23 d\(^{-1}\) with a half-life of 72 h in Skidway River water-sediment slurry (Pritchard 1987); degradation rate constant of 37 \( \mu \)mol L\(^{-1}\) d\(^{-1}\) in freshwater and 22 \( \mu \)mol L\(^{-1}\) d\(^{-1}\) in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990);
- average transformation rate of 53 \( \mu \)mol L\(^{-1}\) d\(^{-1}\) at 31°C for anaerobic degradation in freshwater sediments with an average adaptation time of 37 d (Zhang & Wiegel 1990);
- 70% degradation within 1–2 d in soil and completely degraded within 15 d in river water (NCASI 1992).

Degradation constant \( k = 8.5 \) µM/h for aerobic dechlorination in shake flask experiments; \( k = 10 \) µM/h in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999).
Phenolic Compounds

Biotransformation: microbial transformation rate constant of \((1.7 \pm 0.9) \times 10^{-12} \text{ L organism}^{-1} \text{ h}^{-1}\) (Paris et al. 1982); microbial transformation rate constant of \((4.7 \pm 1.6 \times 10^{-11} \text{ L organism}^{-1} \text{ h}^{-1})\) to \((9.0 \pm 1.7) \times 10^{-11} \text{ L organism}^{-1} \text{ h}^{-1}\) in pond and river samples at five different sites (Paris et al. 1983); degradation rate \(k = 5.44 \times 10^{-17} (\pm 32\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}\) from pure culture studies and \(0.3 \times 10^{-12} \text{ mol cell}^{-1} \text{ h}^{-1}\) with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air: \(t_{1/2} = 1.96 \text{ d in the atmosphere} (\text{Howard 1989})\)

Surface water: \(t_{1/2} = 475 \text{ h for biodegradation in river waters with a calculated first-order rate constant of 0.035 d}^{-1} (\text{Lee & Ryan 1979; quoted, Battersby 1990})\);

\(t_{1/2} = 216–624 \text{ h and 72–1080 h for 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981)}\);

rate constant \(k = 600 \pm 100 \text{ M}^{-1} \text{ s}^{-1}\) for the reaction with ozone at pH 1.5–6.0 (Hoigné & Bader 1983);

\(t_{1/2} = 63 \text{ h in summer at season temp., 25°C, } t_{1/2} = 99 \text{ h in winter at season temp., 14°C in distilled water and 28 h in summer, } t_{1/2} = 63 \text{ h in winter in estuary surface water, based on photo-transformation rate (Hwang et al. 1986)}\);

\(t_{1/2} = 58 \text{ d in summer, } t_{1/2} = 224 \text{ d in winter in distilled water; and } t_{1/2} = 10 \text{ d in summer, } t_{1/2} = 95 \text{ d in winter in surface estuarine water, based on photo-mineralization rate (Hwang et al. 1986)}\);

\(t_{1/2} = 216 \text{ h at 21°C in Skidway River water (Pritchard 1987)}\);

\(t_{1/2} = 20 \text{ d in water (Howard 1989)}\);

at a concentration of 1 mg/L, 4-CP was degraded completely within 15 d in river waters (NCASI 1992); photo-oxidation \(t_{1/2} = 0.4 \text{ min for reaction with Fenton’s reagent; } t_{1/2} = 38.15 \text{ min at pH 2, and } t_{1/2} = 3.4 \text{ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)}\).

Ground water:

Sediment: \(t_{1/2} = 72 \text{ h at 22°C in Skidway River water-sediment slurry (Pritchard 1987)}\);

\(t_{1/2} = 3 \text{ d in sediment and seawater (Howard 1989)}\).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)

\(t_{1/2} = 2.5 \text{ d in an acidic clay soil with } < 1.0\% \text{ organic matter and } t_{1/2} = 1.0 \text{ d in a slightly basic sandy loam soil with 3.25\% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992)}\);

70% degradation with 1 to 2 d (NCASI 1992).

Biota:

TABLE 14.1.2.3.1
Reported aqueous solubilities of 4-chlorophenol at various temperatures

<table>
<thead>
<tr>
<th>Sidgwick &amp; Turner 1922</th>
<th>Achard et al. 1996</th>
<th>Jaoui et al. 1999</th>
<th>Jaoui et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td>synthetic method</td>
<td>shake flask-conductivity</td>
<td>shake flask-optical method</td>
<td>shake flask-optical method*</td>
</tr>
<tr>
<td>(t/\text{°}C)</td>
<td>S/g·m(^{-3})</td>
<td>(t/\text{°}C)</td>
<td>S/g·m(^{-3})</td>
</tr>
<tr>
<td>-0.20</td>
<td>20700</td>
<td>15.1</td>
<td>23337</td>
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<td>65.0</td>
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<td>25.2</td>
<td>25540</td>
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<tr>
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(Continued)
### TABLE 14.1.2.3.1 (Continued)

<table>
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<tr>
<th></th>
<th>Sidgwick &amp; Turner 1922</th>
<th>Achard et al. 1996</th>
<th>Jaoui et al. 1999</th>
<th>Jaoui et al. 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>synthetic method</td>
<td>shake flask-conductivity</td>
<td>shake flask-optical method</td>
<td>shake flask-optical method*</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>T/K</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>T/K</strong></td>
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</tbody>
</table>

Critical solution temp: 129°C
Triple point: -0.30°

*Some data from Achard et al. 1996, Jaoui et al. 1999

**FIGURE 14.1.2.3.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chlorophenol.
TABLE 14.1.2.3.2
Reported vapor pressures of 4-chlorophenol at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
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</tr>
<tr>
<td>136.1</td>
<td>7999</td>
</tr>
<tr>
<td>150.0</td>
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<tr>
<td>172.0</td>
<td>26664</td>
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<tr>
<td>196.0</td>
<td>53329</td>
</tr>
<tr>
<td>220.0</td>
<td>101325</td>
</tr>
</tbody>
</table>

mp/°C  42.0

FIGURE 14.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorophenol.
14.1.2.4  2,4-Dichlorophenol

Common Name: 2,4-Dichlorophenol
Synonym: 2,4-DCP
Chemical Name: 2,4-dichlorophenol
CAS Registry No: 120-83-2
Molecular Formula: C₆H₄Cl₂O, C₆H₃Cl₂OH
Molecular Weight: 163.001

Melting Point (°C):
45.0  (Stull 1947; Verschueren 1977, 1983; Weast 1982–83; Lide 2003)

Boiling Point (°C):
210.0  (Stull 1947; Verschueren 1977, 1983; Weast 1982–83; Lide 2003)

Density (g/cm³):
1.383  (at 60/25 °C, Verschueren 1983)

Acid Dissociation Constant, pKₐ:
7.80  (Blackman et al. 1955; Hoigné & Bader 1983; Scully & Hoigné 1987)
7.85  (Farquharson et al. 1958; Pearce & Simkins 1968)
7.68  (Doedens 1967)
7.89  (Sillén & Martell 1971; Serjeant & Dempsey)
8.01, 8.04, 8.09  (measured values, Xie & Dyrssen 1984)
8.09  (Shigeoka et al. 1988)

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

Enthalpy of Fusion, ΔH₉₄ (kJ/mol):
20.09; 16.7  (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS₉₄ (J/mol K):
Fugacity Ratio at 25 °C (assuming ΔS₉₄= 56 J/mol K), F: 0.636 (mp at 45 °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):
4500  (gravimetric, Mosso 1887)
6194  (shake flask-UV at pH 5.1, Blackman et al. 1955)
5000  (shake flask-spectrophotometry, Roberts et al. 1977)
2650  (shake flask-GC, Jones et al. 1977/1978)
4600  (20°C, Verschueren 1977, 1983)
5547  (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)
4600  (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
5517*  (25.2°C, shake flask-conductimetry, measured range 15.3–35.1°C, Achard et al. 1996)
6339*  (37.35°C, shake flask-optical method, measured range 310.5–423.2 K, Jaoui et al. 1999)
4980  (shake flask-HPLC/UV, pH 4.98, Huang et al. 2000)
4841*  (21.45°C, shake flask-optical method, measured range 296.4–337.7 K, Jaoui et al. 2002)

ln [S/(mol kg⁻¹)] = 11.846 – 3025.1/(T/K); temp range 288–298 K (eq.-I derived using reported exptl. data, Jaoui et al. 2002)
ln [S/(mol kg⁻¹)] = 5.0497 – 981.37/(T/K); temp range 298–347 K (eq.-II derived using reported exptl. data, Jaoui et al. 2002)
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):

20.6* (extrapolated-regression of tabulated data, temp range 53–210°C, Stull 1947)
11.9 (extrapolated-Antoine eq., Weast 1972–73)

\[ \log (P/\text{mmHg}) = [-0.2185 \times 13230.4/(T/\text{K})] + 8.884810; \text{ temp range 53–210°C (Antoine eq., Weast 1972–73)} \]
18.0 (supercooled liquid value, GC-RT correlation, Hamilton 1980)
15.4 (capillary GC-RT, Bidleman & Renberg 1985)
2.40, 11.87 (8°C, 25°C, extrapolated, Leuenberger et al. 1985)

\[ \log (P_1/\text{kPa}) = 6.75941 – 1945.1/(–73.987 + T/\text{K}); \text{ temp range 326–483 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]
\[ \log (P_2/\text{kPa}) = 6.32554 – 1807.32/(–69.17 + T/\text{K}); \text{ temp range 391–474 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

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

0.284 (calculated-P/C, Mabey et al. 1982)
0.110 (8°C, calculated-P/C, Leuenberger et al. 1985)
0.435 (calculated-P/C, Shiu et al. 1994)

\[ k_H/\text{kPa} = 24.9070 – 6791.07/(T/\text{K}); \text{ temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)} \]

0.292 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

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

3.08 (Leo et al. 1971)
3.06 (shake flask-UV, Stockdale & Selwyn 1971)
3.06, 3.08 (Hansch & Leo 1979)
2.92 (HPLC-k’ correlation, Hammers et al. 1982)
3.14 (RP-HPLC-k’ correlation, Miyake & Terada 1982)
3.41 (shake flask-UV, Beltrame et al. 1984)
3.23 (shake flask-HPLC/UV, Schellenberg et al. 1984)
3.21, 3.23 (shake flask-GC, HPLC-k’ correlation, Xie et al. 1984)
3.23 (OECD 1981 guidelines, Leuenberger et al. 1985)
2.87 (RP-HPLC-RT correlation, Chin et al. 1986)
2.97 (HPLC-RT correlation, Miyake et al. 1986)
3.61 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
3.21 (shake flask, Shigeoka et al. 1988; quoted, Saito et al. 1993)
3.16 (shake flask/batch equilibrium-UV, Beltrame et al. 1988)
3.06 (EPA CLOGP Data Base, Hulzebos et al. 1993)
3.17 (recommended, Sangster 1993)
3.07 (calculated-QSAR, Kollig 1993)
3.20 (shake flask-GC, Kishino & Kobayashi 1994)
3.06 (recommended, Hansch et al. 1995)
3.34 (solid-phase microextraction; Dean et al. 1996)

Bioconcentration Factor, log BCF:

1.53 (goldfish, Kobayashi 1979)
1.00 (trout, Hattula et al. 1981)
2.27 (microorganism-water, calculated-K_{ow}, Mabey et al. 1982)
2.00 (golden ide, after 3 d, Freitag et al. 1985)
2.42 (algae, after 1 d, Freitag et al. 1985)
2.53 (activated sludge, after 5 d, Freitag et al. 1985)
1.00 (quoted, brown trout, Walden et al. 1986)
1.80 (correlated, Isnard & Lambert 1988)
1.41–1.65 (estimated, NCASI 1992)
Sorption Partition Coefficient, log $K_{OC}$:

- 2.59 (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
- 2.59–3.02 (soil, calculated-$K_{OW}$, model of Karickhoff et al. 1979, Sabljic 1987a,b)
- 2.89–3.12 (soil, calculated-$K_{OW}$, model of Kenaga & Goring 1980, Sabljic 1987a,b)
- 2.10–2.32 (soil, calculated-$K_{OW}$, model of Briggs 1981, Sabljic 1987a,b)
- 2.48–2.91 (soil, calculated-$K_{OW}$, model of Means et al. 1982, Sabljic 1987a,b)
- 1.74–2.13 (soil, calculated-$K_{OW}$, model of Chiou et al. 1983, Sabljic 1987a,b)
- 3.60, 3.50 (untreated fine and coarse sediment, Isaacson & Frink 1984)
- 3.71, 3.98 (treated fine and coarse sediment, Isaacson & Frink 1984)
- 2.75 (sediment, Schenllenberg et al. 1984; quoted, Sabljic 1987a,b)
- 2.49 (calculated-$K_{OW}$, Kollig 1993)
- 2.75 (soil, calculated-$MCI\chi$, Sabljic et al. 1995)
- 2.47, 2.53 (RP-HPLC-$k'$ correlation including $MCI$ related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.49, 2.57, 2.77, 2.33 (soils: organic carbon $OC$ -0.1% and pH 2.0–7.4, $OC$ –0.1% and pH $\leq 5.8$, $OC$ –0.5%, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis:

- $k_P = 0.82$ h$^{-1}$ with $t_{1/2} = 0.8$ h for distilled water in summer at mean temp. 25°C, and $k_P = 0.21$ h$^{-1}$ with $t_{1/2} = 3$ h in winter at mean temp. 11°C; $k_P = 1.16$ h$^{-1}$ with $t_{1/2} = 0.6$ h for estuarine water in summer and $k_P = 0.44$ h$^{-1}$ with $t_{1/2} = 2$ h in winter; $k_P = 1.0$ h$^{-1}$ with $t_{1/2} = 0.7$ h in summer and $k_P = 0.38$ h$^{-1}$ with $t_{1/2} = 2$ h in winter for poisoned estuarine water when exposed to full sunlight and microbes (phototransformation, Hwang et al. 1986)
- $k_P = 0.09$ h$^{-1}$ with $t_{1/2} = 8$ d in summer and $k_P = 0.049$ h$^{-1}$ with $t_{1/2} = 14$ d in winter for distilled water; $k_P = 0.20$ h$^{-1}$ with $t_{1/2} = 4$ d in summer and $k_P = 0.04$ h$^{-1}$ with $t_{1/2} = 17$ d in winter for estuarine water; $k_P = 0.12$ h$^{-1}$ with $t_{1/2} = 6$ d in summer and $k_P = 0.05$ h$^{-1}$ with $t_{1/2} = 14$ d in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-mineralization rate, Hwang et al. 1986)
- photochemical-transformation $t_{1/2} = 2.5–2.6$ h in Xenotest 1200 (Svenson & Björndal 1988)
- atmospheric and aqueous photolysis $t_{1/2} = 0.8–3$ h based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991)
- $k_P = 38 \times 10^3$ min$^{-1}$ with a $t_{1/2} = 17.5$ min for direct UV radiation aqueous solutions (Benitez et al. 2000)

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

- $k < 7 \times 10^3$ M$^{-1}$ h$^{-1}$ for singlet oxygen, and $1 \times 10^7$ M$^{-1}$ h$^{-1}$ for peroxo radical at 25°C (Mabey et al. 1982)
- $k = 5 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 8, $k < 1.5 \times 10^3$ M$^{-1}$ s$^{-1}$ for non-protonated species, $k = (8 \pm 4) \times 10^9$ M$^{-1}$ s$^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM t-BuOH as scavenger at pH 1.3–1.5 and 20–23°C (Hoigné & Bader 1983b)
- $k = 7 \times 10^5$ M$^{-1}$ s$^{-1}$ at pH 5.5, $k = 2 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 6.0, $k = 10 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 6.6, $k = 15 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 7.0, $k = 76 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 7.9, $k = 120 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 9.0 and pH 9.6 for the reaction with singlet oxygen in water at 19 ± 2°C (Scully & Hoigné 1987)
- $k_{OH} = 1.06 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1989)
- $k_{OH} = 3.5 \times 10^{-12}$ cm$^3$ molecule s$^{-1}$ (Bunce et al. 1991)
- $k = (5.1 \pm 4.7) \times 10^6$ M$^{-1}$ s$^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at 27 ± 1°C (Tratnyek & Hoigné 1991)
- $k_{OH(calc)} = 1.71 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital estimation method, Klamt 1993)
- $k = 209 \times 10^3$ min$^{-1}$ with a half-life of 2.4 min for reaction with Fenton’s reagent; and $k = 24 \times 10^3$ min$^{-1}$ with a half-life of 30.4 min at pH 2, and $k = 315 \times 10^3$ min$^{-1}$ with a half-life of 3.3 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: 7 to 10 d for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964);
aqueous aerobic $t_{1/2} = 66.7–199$ h, based on aerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 324–1032$ h, based on anaerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991); completely degraded in soil suspensions in 9 d (Woodcock 1971; quoted, Verschueren 1983); average rate of biodegradation 10.5 mg COD g$^{-1}$ h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); aerobic degradation in a non-sterile clay-loam soil: 79% loss at 0°C at the termination of the experiment after 14 days, 82% loss at 4°C after 12 d and 84% loss at 20°C after 40 d all under same experimental conditions (Baker et al. 1980); rate constants $k = 0.5$ d$^{-1}$ with $t_{1/2} = 1.4$ d in adapted activated sludge and $k = 0.1$ d$^{-1}$ with $t_{1/2} = 6$ d in natural waters under anaerobic conditions (Mills et al. 1982); microbial degradation negligible in darkness (Hwang et al. 1986); $k = 0.223$ h$^{-1}$ for maximum removal by activated sludge microorganisms (Chudoba et al. 1989); biodegradation first-order rate of hydroxylation, $k = 0.017$ min$^{-1}$ by pseudomonas putida Fl (Spain et al. 1989; quoted, Neilson et al. 1991); 15% reduction in concn (2 $\mu$M) after incubation with cells of Rhodococcus chlorophenolicus for 14 d under aerobic conditions (Neilson et al. 1991) transformation rate of 245 -mol L$^{-1}$ d$^{-1}$ at 31°C for anaerobic degradation in freshwater sediments with an average of 7 d adaptation time (Zhang & Wiegel 1990); complete biodegradation in water, seawater, sludge and lagoon within 16 to 23 d (NCASI 1992). Degradation constant $k = 1.6$ $\mu$M/h for anaerobic batch experiment in serum bottles; $k = 1.2$ $\mu$M/h for dechlorination in anaerobic batch or continuous bioreactor; $k = 1.9$ $\mu$M/h in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999) Biotransformation: for bacterial transformation $k = 1 \times 10^7$ mL cell$^{-1}$ h$^{-1}$ in water (Mabey et al. 1982); degradation rate $k = 3.76 \times 10^{-19}$ mol cell$^{-1}$·h$^{-1}$ (± 47% SD) from pure culture studies, $k = 0.02 \times 10^{-14}$ to $2 \times 10^{-14}$ mol cell$^{-1}$·h$^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 3 d for reaction with OH radical on March 21 at 43°N; lifetime varies from 2 to 20 d at the latitude of Toronto depending on seasons; at latitude of 43.7°N, tropospheric lifetimes are: 20 d on December 21, 5 d on February 21, 2.2 d on April 21 and 1.5 d on June 21; and at different geographical locations on March 21, lifetimes are 1.7 d at latitude 0°, 2.2 d at 25°S, 6.7 d at 55°S and 680 at 85°S (Bunce et al. 1991); $t_{1/2} = 21.2–212$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991). Surface water: rate constant $k < 1.5 \times 10^3$ M$^{-1}$ s$^{-1}$ for the reaction with ozone at pH 1.5–3.0 (Hoigné & Bader 1983); $t_{1/2} = 0.8$ h in summer, $t_{1/2} = 3.0$ h in winter for distilled water; $t_{1/2} = 0.7$ h in summer, $t_{1/2} = 2.0$ h in winter for poisoned estuarine water; $t_{1/2} = 0.6$ h in summer, $t_{1/2} = 2.0$ h in winter for estuarine water, all based on photo-transformation rate under full sunlight and microbes; $t_{1/2} = 8.0$ d in summer, $t_{1/2} = 14$ d in winter for distilled water; $t_{1/2} = 6$ d in summer, $t_{1/2} = 14$ d in winter for poisoned estuarine water and $t_{1/2} = 4$ d in summer, $t_{1/2} = 17$ d in winter for estuarine water, based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986); $t_{1/2} = 62$ h in water at pH 8 and 19 ± 2°C for the reaction with singlet oxygen (Scull & Hoigné 1987); $t_{1/2} = 2.5–2.6$ h for photochemical transformation in Xenotest 1200 (Svensson & Björndal 1988); $t_{1/2} = 0.8–3$ h based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991); complete biodegradation within 5–23 d in seawater (NCASI 1992); photo-oxidation $t_{1/2} = 2.4$ min for reaction with Fenton’s reagent; $t_{1/2} = 30.4$ min at pH 2 and $t_{1/2} = 3.3$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000). Ground water: $t_{1/2} = 133–1032$ h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991). Sediment: mean half-life of dechlorination: $t_{1/2} = 116$ d in July and $t_{1/2} = 47$ d in November (Hale et al. 1991). Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)
t_{1/2} = 176–1680 h, based on aerobic soil die-away test data (Baker et al. 1980; Haider et al. 1974; selected, Howard et al. 1991);
t_{1/2} = 3.5 d in an acidic clay soil with < 1.0% organic matter and 1.5 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

### TABLE 14.1.2.4.1
Reported aqueous solubilities and vapor pressures of 2,4-dichlorophenol at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Achard et al. 1996</td>
<td>Jaoui et al. 1999</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>T/K</td>
</tr>
<tr>
<td>------</td>
<td>---------</td>
<td>-----</td>
</tr>
<tr>
<td>15.3</td>
<td>3896</td>
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<td>25.2</td>
<td>5517</td>
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<td>38.2</td>
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<td>401.5</td>
</tr>
<tr>
<td>42.3</td>
<td>15394</td>
<td>408.4</td>
</tr>
</tbody>
</table>

*some data from Achard et al. 1996, Jaoui et al. 1999

FIGURE 14.1.2.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2,4-dichlorophenol.
FIGURE 14.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dichlorophenol.

- b.p. = 210 °C
- m.p. = 45 °C

Stull 1947
14.1.2.5 2,6-Dichlorophenol

Common Name: 2,6-Dichlorophenol
Synonym: 2,6-DCP
Chemical Name: 2,6-dichlorophenol
CAS Registry No: 87-65-0
Molecular Formula: C₆H₃Cl₂OH
Molecular Weight: 163.001
Melting Point (°C):
68.5  (Lide 2003)
Boiling Point (°C):
220  (Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
6.91  (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)
6.80  (Doedens 1967; McLeese et al. 1979)
6.79  (Pearce & Simkins 1968)
6.79  (Sillén & Martell 1971; Kaiser et al. 1984; Xie & Dyrrsen 1984; Shigeoka et al. 1988)
6.78  (Ugland et al. 1981; Dean 1985)
6.54  (Nendza & Seydel 1988)
Molar Volume (cm³/mol):
145.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔHₚₑᵤ₃ (kJ/mol):
22.14  (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₚₑᵤ₃ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₑᵤ₃ = 56 J/mol·K), F: 0.374 (mp at 68.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
2625  (shake flask-HPLC/UV at pH 4.5, Ma et al. 1993)
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):
13.1*  (extrapolated-regression of tabulated data, temp range 59.5–220°C, Stull 1947)
12.9  (extrapolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 13472.0/(T/K)] + 8.864007; temp range 59.5–220°C (Antoine eq., Weast 1972–73)
12.2  (supercooled liq. value, GC-RT correlation, Hamilton 1980)
12.7  (capillary GC-RT, Bidleman & Renberg 1985)
11.2  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P(Π)/kPa) = 7.32845 – 2436.59/(–35.584 + T/K); temp range 333–493 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P(Π)/kPa) = 5.2254 – 1106.4/(–151.42 + T/K); temp range 353–493 K (Antoine eq.-II, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.7376  (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, log Kₒₒₜₕ:
2.86  (Hansch & Leo 1979)
2.34  (HPLC-RT correlation, Butte et al. 1981)
2.64  (HPLC-k' correlation, Hammers et al. 1982)
Phenolic Compounds

3.36 (shake flask-UV, Beltrame et al. 1984)
2.84, 2.92 (shake flask-GC, HPLC-k’ correlation, Xie et al. 1984)
2.84 (shake flask, Shigeoka et al. 1988)
2.80 (batch equilibration-UV, Beltrame et al. 1988)
2.64 (recommended, Sangster 1993)
2.92 (shake flask-GC, Kishino & Kobayashi 1994)
2.75 (recommended, Hansch et al. 1995)
2.57 (HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, log BCF:
1.44–1.56 (estimated, NCASI 1992)

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants and Half-Lives:

Vaportilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation: 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments respectively (de Kreuk & Hanstveit 1981)
81% reduction in concn (2 µM) after incubation with cells of Rhodococcus chlorophenolicus for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:
Bioconcentration Uptake (kJ1) and Elimination (kJ3) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: t½ = 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments, respectively (de Kreuk & Hanstveit 1981).

Ground water:
Sediment:
Soil: t½ = 16.2 d in an acidic clay soil with < 1.0% organic matter and t½ = 2.4 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.5.1
Reported vapor pressures of 2,6-dichlorophenol at various temperatures

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>59.5</td>
<td>133.3</td>
</tr>
<tr>
<td>87.5</td>
<td>666.6</td>
</tr>
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<td>101.0</td>
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<td>115.5</td>
<td>2666</td>
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<td>131.5</td>
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<td>141.8</td>
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<td>154.6</td>
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<td>175.5</td>
<td>26664</td>
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<td>197.7</td>
<td>53329</td>
</tr>
<tr>
<td>220.0</td>
<td>101325</td>
</tr>
<tr>
<td>mp/°C</td>
<td></td>
</tr>
</tbody>
</table>

(Stull 1947)

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FIGURE 14.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dichlorophenol.
14.1.2.6  3,4-Dichlorophenol

![Structure of 3,4-Dichlorophenol](image)

Common Name: 3,4-Dichlorophenol  
Synonym: 3,4-DCP  
Chemical Name: 3,4-dichlorophenol  
CAS Registry No: 95-77-2  
Molecular Formula: C₆H₃Cl₂OH  
Molecular Weight: 163.001  
Melting Point (°C): 68.0 (Weast 1982–83; Lide 2003)  
Boiling Point (°C): 253 (Lide 2003)  
Density (g/cm³):  
Acid Dissociation Constant, pKₐ:  
  7.39 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)  
  8.59 (Pearce & Simkins 1968; Serjeant & Dempsey 1979; Hammers et al. 1982)  
  8.59 (Sillén & Martell 1971; Kaiser et al. 1984)  
  8.68 (Xie & Dyrssen 1984; Shigeoka et al. 1988; Sangster 1993)  
  8.63 (Dean 1985)  
Molar Volume (cm³/mol): 145.2 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ∆H_{fus} (kJ/mol): 20.93 (exp., Chickos et al. 1999)  
Entropy of Fusion, ∆S_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol·K), F: 0.379 (mp at 68°C)  
Water Solubility (g/m³ or mg/L at 25°C): 9256 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)  
Vapor Pressure (Pa at 25°C):  
Henry’s Law Constant (Pa·m³/mol):  
Octanol/Water Partition Coefficient, log K_{ow}:  
  3.37 (Hansch & Leo 1979)  
  3.05 (HPLC-k’ correlation, Hammers et al. 1982)  
  3.33 (HPLC-RT correlation, Banerjee et al. 1984)  
  3.47 (shake flask-UV, Beltrame et al. 1984)  
  3.44, 3.41 (shake flask-GC, HPLC-k’ correlation, Xie et al. 1984)  
  3.44 (shake flask, Shigeoka et al. 1988)  
  3.68 (shake flask/batch equilibration-UV, Beltrame et al. 1988)  
  3.33 (recommended, Sangster 1993)  
  3.27; 3.39 (HPLC-RT correlation; electrometric titration, Slater et al. 1994)  
  3.33 (recommended, Hansch et al. 1995)  
Bioconcentration Factor, log BCF:  
  1.43, 1.38 (earthworm E. fetida andreii: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)  
  1.30, 1.61 (earthworm L. rubellus: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
1.79, 1.8, 1.94, 2.04 (earthworm system, collated from literature, Connell & Markwell 1990)
0.8, 1.3, 1.4, 1.80 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, log $K_{OC}$:
3.09 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
3.03 (2.93–3.13) (soil: organic carbon $OC \geq 0.5\%$ and $pH \leq 6.0$, average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:
Volatilization:
Photolysis:
oxidation:
Hydrolysis:
Biodegradation: biodegradation first-order rate of hydroxylation of 0.008 min$^{-1}$ by Pseudomonas putida Fl (Spain et al. 1989; quoted, Neilson et al. 1991).
Biotransformation: degradation rate of $6.84 \times 10^{-19}$ (± 38% SD) mol cell$^{-1}$ h$^{-1}$ from pure culture studies (Banerjee et al. 1984).

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

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment: mean half-life of dechlorination: $t_{1/2} = 115$ d in July and $t_{1/2} = 86$ d in November with relatively long $t_{1/2} = 66$ d reported from site 1, $t_{1/2} = 64$ d from site 3 and $t_{1/2} = 132$ d from site 5 in January (Hale et al. 1991).
Soil: disappearance $t_{1/2} = 10.1$ d from Kooyenburg soil, $t_{1/2} = 11.2$ d from Holten soil with earthworms E. fetida andrei and $t_{1/2} = 24.7$ d from Kooyenburg soil, $t_{1/2} = 49.5$ d from Holten soil with earthworms L. rebellus (van Gestel & Ma 1988);
$t_{1/2} = 18.3$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 3.2$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab experiments (Loehr & Matthews 1992).
Biota:
14.1.2.7 2,3,4-Trichlorophenol

Common Name: 2,3,4-Trichlorophenol
Synonym:
Chemical Name: 2,3,4-trichlorophenol
CAS Registry No: 1595-06-0
Molecular Formula: C₆H₃Cl₃O, C₆H₂Cl₃OH
Molecular Weight: 197.446
Melting Point (°C):
  83.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  sublimation (Weast 1982–83; Dean 1985; Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
  7.66 (Doedens 1967)
  6.50 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984; Shigeoka et al. 1988; Sangster 1993)
  6.97 (Ugland et al. 1981; Dean 1985; Renner 1990; Ma et al. 1993)
  7.18 (Schellenberg et al. 1984)
Molar Volume (cm³/mol):
  166.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol·K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol·K), F: 0.267 (mp at 83.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
  500 (estimated, Ma et al. 1990)
  915 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)
Vapor Pressure (Pa at 25°C):
  1.00 (selected, Ma et al. 1990)
  3.48 (selected P_L, Shiu et al. 1994)
Henry’s Law Constant (Pa·m³/mol):
  0.3959 (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, log K_{OW}:
  4.07 (Hansch & Leo 1979)
  3.51 (HPLC-RT correlation, Butte et al. 1981)
  3.54 (HPLC-k’ correlation, Hammers et al. 1982)
  3.80 (shake flask-UV, Beltrame et al. 1984)
  3.80 (shake flask, Shigeoka et al. 1988)
  3.82 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
  3.61 (recommended, Sangster 1993)
  3.51, 3.54, 3.80 (lit. values, Hansch et al. 1995)
Bioconcentration Factor, log BCF:

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

Environmental Fate Rate Constants and Half-Lives:
  Volatilization:
   Photolysis: photochemical-transformation $t_{1/2} = 1.7$ h in Xenotest 1200 (Svenson & Björndal 1988).
  Photooxidation:
  Hydrolysis:
  Biodegradation:
  Biotransformation:
  Bioconcentration Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
  Air:
   Surface water: 1.7 h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).
  Ground water:
  Sediment:
  Soil:
  Biota:
14.1.2.8 2,4,5-Trichlorophenol

Common Name: 2,4,5-Trichlorophenol
Synonym: 245-TCP
Chemical Name: 2,4,5-trichlorophenol
CAS Registry No: 95-95-4
Molecular Formula: C₆H₂Cl₃OH
Molecular Weight: 197.446
Melting Point (°C):
   69  (Lide 2003)
Boiling Point (°C):
   247 (Lide 2003)
Density (g/cm³ at 20°C):
   1.500  (75°C, Verschueren 1983)
Acid Dissociation Constant, pKₐ:
   7.00  (Blackman et al. 1955, Sillén & Martell 1971; Kaiser et al. 1984)
   7.07  (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)
   7.43  (Doedens 1967; Jones 1981; Bintein & Devillers 1994)
   6.72  (Ugland et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)
   6.90  (Hoigné & Bader 1983)
   6.94  (Schellenberg et al. 1984; Sangster 1993)
   6.83  (Nendza & Seydel 1988)
Molar Volume (cm³/mol):
   166.1  (calculated-Le Bas method at normal boiling point)
   165.5  (calculated-χ, Sabljic 1987b)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
   21.59  (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₚ = 56 J/mol K), F: 0.370 (mp at 69°C)
Water Solubility (g/m³ or mg/L at 25°C):
   948  (shake flask-UV at pH 5.1, Blackman et al. 1955)
   990  (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)
   700  (8°C, Leuenberger et al. 1985)
   649  (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)
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):
   6.69*  (extrapolated-regression of tabulated data, temp range 72–251.8°C, Stull 1947)
   6.60  (extrapolated liquid value, Antoine eq. Weast 1972–73)
   log (P/mmHg) = [–0.2185 × 13237.0/(T/K)] + 8.401072; temp range 72–251.8°C (Antoine eq., Weast 1972–73)
   6.12  (supercooled liquid, GC-RT correlation, Hamilton 1980)
   2.66  (capillary GC-RT, Bidleman & Renberg 1985)
   2.93  (selected, Leuenberger et al. 1985)
   7.64  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
   log (P/kPa) = 7.38179 – 2812.25/(–2.091 + T/K); temp range 345–525 K (Antoine eq., Stephenson & Malanowski 1987)
   2.93  (calculated, Howard 1991)
Henry's Law Constant (Pa·m³/mol at 25°C):

0.132 (8°C, Leuenberger et al. 1985)
0.590 (calculated, Howard 1991)
0.521 (calculated-P/C, Shiu et al. 1994)

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

3.72 (Leo et al. 1971; Hansch & Leo 1979; 1982)
2.39 (estimated-HPLC-RT correlation, Veith et al. 1979)
3.63 (HPLC-k’ correlation, Hammers et al. 1982)
3.80 (shake flask-GC, Saarikoski & Viluksela 1982)
4.19 (shake flask-HPLC/UV, Schellenberg et al. 1984)
4.10, 3.96 (shake flask-GC, HPLC-k’ correlation, Xie et al. 1984)
3.73 (HPLC-RT correlation, Miyake et al. 1986)
3.84 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
4.10 (shake flask, Shigeoka et al. 1988)
3.72 (recommended, Sangster 1993)
4.02 (shake flask-GC, Kishino & Kobayashi 1994)
3.72 (recommended, Hansch et al. 1995)
3.83 (HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, log BCF:

3.28 (fathead minnow-28 d exposure, Veith et al. 1979b)
3.28, 2.70 (total $^{14}$C in fathead minnows, observed, calculated, mean exposure level 0.0048 µg·mL⁻¹, Call et al. 1980)
3.26, 2.82 (total $^{14}$C in fathead minnows, observed, calculated, mean exposure level 0.0493 µg·mL⁻¹, Call et al. 1980)
3.27 (total $^{14}$C in fathead minnows, mean value, Call et al. 1980)
2.40 (calculated-$K_{ow}$, Mackay 1982)
2.88 (calculated-MCI $\chi$, Sabljic 1987a)
1.79 (fish, van Gestel & Ma 1988)
1.81, 1.53 (earthworms E. fetida andreii: Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.82 (earthworms L. rubellus: Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.39, 2.61, 3.36 (earthworm system, collated from literature, Connell & Markwell 1990)
0.40, 1.50, 2.50, 8.40 (earthworm system, derived data, Connell & Markwell 1990)
3.28; 3.61 (fathead minnows; fish, Howard 1991)
2.14 (estimated, NCASI 1992)

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

3.49–3.98 (soil, calculated-$K_{ow}$ model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.38–3.64 (soil, calculated-$K_{ow}$ model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.56–2.82 (soil, calculated-$K_{ow}$ model of Briggs 1981, Sabljic 1987a,b)
3.38–3.87 (soil, calculated-$K_{ow}$ model of Means et al. 1982, Sabljic 1987a,b)
2.55–2.99 (soil, calculated-$K_{ow}$ model of Chiou et al. 1983, Sabljic 1987a,b)
3.36 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
2.99 (soil, calculated-MCI $\chi$, Sabljic 1987a,b)
3.25, 3.12, 3.38, 2.56 (quoted:lake sediment, river sediment, aquifer material, soil, Howard 1991)
3.34, 3.30 (soils, Howard 1991)
2.93 (calculated-$K_{ow}$, Kollig 1993)
3.36 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
3.11 (2.81–3.41), 3.35 (3.30–3.40) (soils: organic carbon OC $\geq$ 0.1% and pH 3.4–6.0, OC $\geq$ 0.5% and pH $\leq$ 4.9 undissociated, average, Delle Site 2001)
Phenolic Compounds

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

Volatile: volatilization t½ ~ 9.0 d from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s, and t½ = 207 d from a model pond (Howard 1991).

Photolysis:

\[ k_p = 1.30 \text{ h}^{-1} \text{ with } t_{1/2} = 0.6 \text{ h in summer \ and \ at \ mean \ temp. \ 25°C \ and } k_p = 0.61 \text{ h}^{-1} \text{ with } t_{1/2} = 1.0 \text{ h in winter \ at \ mean \ temp \ 18°C \ in \ distilled \ water; } k_p = 1.20 \text{ h}^{-1} \text{ with } t_{1/2} = 0.6 \text{ h in summer \ and } k_p = 0.65 \text{ h}^{-1} \text{ with } t_{1/2} = 1.0 \text{ h in winter \ for \ estuarine \ water \ under \ full \ sunlight \ and \ microbes (photo-transformation, Hwang et al. 1986) } \]

\[ k_p = 1.30 \text{ h}^{-1} \text{ corresponding to a } t_{1/2} = 0.5 \text{ h in summer, } k_p = 0.61 \text{ h}^{-1} \text{ corresponding to a } t_{1/2} = 1.0 \text{ h in winter \ in \ distilled \ water \ and } k_p = 1.20 \text{ h}^{-1} \text{ corresponding to a } t_{1/2} = 0.6 \text{ h in summer, } k_p = 0.65 \text{ h}^{-1} \text{ corresponding to a } t_{1/2} = 1.0 \text{ h in winter \ in \ estuarine \ water \ under \ irradiation \ by \ natural \ sunlight \ (quoted \ from \ Hwang \ et \ al. 1987, Sanders et al. 1993) } \]

\[ t_{1/2} = 0.5–336 \text{ h, based on photolysis rate constants \ for \ transformation \ and \ mineralization \ under \ summer \ and \ winter, \ sunlight \ conditions (Howard \ et \ al. 1991) } \]

\[ \text{photolysis } t_{1/2} = 0.6 \text{ and } 1.0 \text{ h in natural water (and \ distilled \ water) \ exposed \ to \ midday \ sunlight \ during \ summer \ and \ winter \ respectively (Howard 1991) } \]

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

\[ k(aq.) > 10^9 \text{ M}^{-1} \text{ s}^{-1} \text{ at pH 8, and } k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for non-protonated species, } k > 10^9 \text{ M}^{-1} \text{ s}^{-1} \text{ for phenolate ions for the reaction with ozone in water using 3 mM t-BuOH as scavenger at pH 1.2–1.5 and 20–23°C (Hoigné & Bader 1983b) } \]

\[ k_{OH} = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule s}^{-1} \text{ (Bunce et al. 1991) } \]

Hydrolysis: t½ > 8 × 10^6 yr, based on hydrolysis rate constant is zero at pH 7.0 (Kollig et al. 1987; selected, Howard et al. 1991).

Biodegradation: decomposition in suspended soils: > 72 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983);

\[ 840 \text{ h for 75% degradation \ in \ mineral \ medium (de Kreuk & Hanstveit 1981); } \]

\[ \text{aqueous aerobic } t_{1/2} = 552–16560 \text{ h, based on unacclimated aerobic river die-away test data (Lee & Ryan 1979; selected, Howard et al. 1991); aqueous anaerobic } t_{1/2} = 3028–43690 \text{ h, based on unacclimated anaerobic grab sample data for soil and ground water (Gibson & Sufita 1986; Baker & Mayfield 1980; selected, Howard et al. 1991); } \]

\[ \text{degradation with microbes in darkness negligible (Hwang et al. 1986); degradation } k = 0.00010 \text{ d}^{-1} \text{ with a } t_{1/2} = 16560 \text{ h and } k = 0.030 \text{ d}^{-1} \text{ with a } t_{1/2} = 552 \text{ h for Skidway River water and water-sediment slurry, respectively (Pritchard 1987); biodegradation } t_{1/2} = 690 \text{ d in river water (Howard 1991) } \]

\[ 70\% \text{ reduction in concn (2 } \mu\text{M) after incubation with cells of } \text{Rhodococcus chlorophenolicus \ for \ 14 \ d under aerobic \ conditions (Neilson et al. 1991) } \]

\[ t_{1/2(\text{aerobic})} = 25 \text{ d, } t_{1/2(\text{anaerobic})} = 130 \text{ d in natural waters (Capel & Larson 1995) } \]

Biotransformation: degradation rate k = 1.43 × 10^{-20} (± 77% SD) mol cell^{-1} h^{-1} from pure culture studies and k = 5 × 10^{-15} mol cell^{-1} h^{-1} with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air: tropospheric lifetime of 4 d on March 21 at 43°N (Bunce et al. 1991);

\[ t_{1/2} = 30.1–301 \text{ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991); } \]

\[ t_{1/2} < 7.5 \text{ d for reactions with OH radical (estimated, Howard 1991); atmospheric transformation lifetime was estimated to be } > 5 \text{ d (Kelly et al. 1994). } \]

Surface water: 840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

\[ \text{Rate constant } k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with } O_3 \text{ at pH 1.2–1.5 (Hoigné & Bader 1983); } \]

\[ t_{1/2} = 0.5 \text{ h (summer), } t_{1/2} = 1.0 \text{ h (winter) in distilled water and } t_{1/2} = 0.5 \text{ h (summer), } t_{1/2} = 1.0 \text{ h (winter) in surface estuarine water based on photo-transformation rate under full sunlight and microbes (Hwang et al. 1986); } \]
\( t_{1/2} = 7 \text{ d (summer)} \), \( t_{1/2} = 14 \text{ d (winter)} \) in distilled water and \( t_{1/2} = 3 \text{ d (summer)} \), \( t_{1/2} = 8 \text{ d (winter)} \) in estuarine water based on photo-mineralization rater under full sunlight and microbes (Hwang et al. 1986);

\( t_{1/2} = 0.6 \text{ h (summer)} \), \( t_{1/2} = 1.0 \text{ h (winter)} \) in poisoned estuarine water based on photo-transformation rate and

\( t_{1/2} = 6 \text{ d (summer)} \), \( t_{1/2} = 14 \text{ d (winter)} \) in poisoned estuarine water based on photomineralization rate (Hwang et al. 1986);

\( t_{1/2} = 16560 \text{ h at 21°C in Skidway River water} \) (Pritchard 1987);

photodegradation \( t_{1/2} = 0.5 \text{ h (summer)} \), \( t_{1/2} = 1.0 \text{ h (winter)} \) in distilled water and \( t_{1/2} = 0.6 \text{ h (summer)} \), \( t_{1/2} = 1.0 \text{ h (winter)} \) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993);

\( t_{1/2} = 0.5–336 \text{ h, based on aqueous photolysis half-life} \) (Howard et al. 1991); rapidly photolyze with a

\( t_{1/2} = 0.6–1.0 \text{ h at water surfaces, } t_{1/2} = 690 \text{ d in water column} \) (Howard 1991)

\( t_{2(aerobic)} = 25 \text{ d, } t_{2(anaerobic)} = 130 \text{ d in natural waters} \) (Capel & Larson 1995)

Ground water: \( t_{1/2} = 1104–43690 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life} \) (Howard et al. 1991).

Sediment: \( t_{1/2} = 23 \text{ d from calculated degradation rate constant } k = 0.0030 \text{ d}^{-1} \) for radiolabeled 2,4,5-TCP in Skidway River water-sediment slurry (Lee & Ryan 1979; quoted, Pritchard 1987);

biodegradation \( t_{1/2} = 23 \text{ d in sediments} \) (Howard 1991).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961)

disappearance \( t_{1/2} = 3.4 \text{ d from Kooyenburg soil and } t_{1/2} = 6.6 \text{ d from Holten soil with earthworms } E. \text{ fetida andrei} \)

and \( t_{1/2} = 39.6 \text{ d from Kooyenburg soil, } t_{1/2} = 13.9 \text{ d from Holten soil with earthworm } L. \text{ rubellus} \)

(van Gestel & Ma 1988);

\( t_{1/2} = 33 \text{ d in sandy loam} \) (Kjeldsen et al. 1990)

\( t_{1/2} = 552–16560 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life} \) (Howard et al. 1991);

under aerobic conditions biodegradation \( t_{1/2} = 15 \text{ d in a soil suspension} \) (Howard 1991);

\( t_{1/2} = 22.3 \text{ d in an acidic clay soil with } <1.0\% \text{ organic matter and } t_{1/2} = 14.6 \text{ d in a slightly basic sandy loam soil with } 3.25\% \text{ organic matter, based on aerobic batch lab microcosm experiments} \) (Loehr & Matthews 1992).

Biota: depuration \( t_{1/2}(\text{obs.}) = 12 \text{ h, } t_{1/2}(\text{calc}) = 9.2 \text{ h for mean exposure level of 0.0048 } \mu \text{g·mL}^{-1} \) and \( t_{1/2}(\text{obs.}) = 12 \text{ h, } t_{1/2}(\text{calc}) = 6.6 \text{ h for mean exposure level of 0.0493 } \mu \text{g·mL}^{-1} \) (fathead minnow, Call et al. 1980).

<table>
<thead>
<tr>
<th>TABLE 14.1.2.8.1</th>
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<tbody>
<tr>
<td>Reported vapor pressures of 2,4,5-trichlorophenol at various temperatures</td>
</tr>
</tbody>
</table>

**Stull 1947**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/\text{Pa} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>72.0</td>
<td>133.3</td>
</tr>
<tr>
<td>102.1</td>
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<tr>
<td>117.3</td>
<td>1333</td>
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<td>162.5</td>
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<tr>
<td>178.0</td>
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<tr>
<td>201.5</td>
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<td>226.5</td>
<td>53329</td>
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<tr>
<td>251.8</td>
<td>101325</td>
</tr>
<tr>
<td>mp/°C</td>
<td>62</td>
</tr>
</tbody>
</table>

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**FIGURE 14.1.2.8.1** Logarithm of vapor pressure versus reciprocal temperature for 2,4,5-trichlorophenol.
14.1.2.9  2,4,6-Trichlorophenol

Common Name: 2,4,6-Trichlorophenol
Synonym: 2,4,6 TCP
Chemical Name: 2,4,6-trichlorophenol
CAS Registry No: 88-06-2
Molecular Formula: C₆H₂Cl₃OH
Molecular Weight: 197.446
Melting Point (°C):
   69  (Lide 2003)
Boiling Point (°C):
   246.0  (Stull 1947; Weast 1982–83; Lide 2003)
Density (g/cm³):
   1.675  (Schmidt-Bleek et al. 1982)
   1.491  (75°C, Weast 1982–83)
Acid Dissociation Constant, pKₐ:
   6.10  (Blackman et al. 1955)
   6.22  (Farquharson et al. 1958; Saarikoski & Viluksela 1982)
   5.99  (Dean 1985)
   6.23  (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991)
   6.00  (Xie 1983, Yoshida et al. 1987)
   6.15  (Schellenberg et al. 1984; Leuenberger et al. 1985)
   6.18  (Sangster 1993)
Molar Volume (cm³/mol):
   166.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.370 (mp at 69°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):

858  (gravimetric method, Daccomo 1885)
434  (shake flask-UV at pH 5.1, Blackman et al. 1955)
900  (shake flask-spectrophotometry, Roberts et al. 1977)
430  (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)
312  (20°C, phenol form, shake flask-HPLC/UV, Yoshida et al. 1987)
312 × (1 + 10^{0.6-6.06})  (20°C, measured at pH 4, 5, 6 and 7, shake flask-HPLC/UV, Yoshida et al. 1987)
300, 580, 270000  (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)
708  (shake flask-HPLC/UV at pH 4.7, Ma et al. 1993)
800  (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
692*  (24.9°C, shake flask-conductimetry, measured range 19.5–30.0°C, Achard et al. 1996)
1144*  (41.05°C, shake flask-optical method, measured range 314.2–420.6 K, Jaoui et al. 1999)
503  (shake flask-HPLC/UV, pH 5.03, Huang et al. 2000)
439.6*  (21.75°C, shake flask-optical method, measured range 294.9–318.2 K, Jaoui et al. 2002)
ln [S/(mol kg⁻¹)] = 23.367 – 7096.7/(T/K); temp range 292–303 K (eq. derived using reported explt. data, Jaoui et al. 2002)
ln [S/(mol kg⁻¹)] = 6.6069 – 2029.9/(T/K); temp range 303–334 K (eq. derived using reported explt. data, Jaoui et al. 2002)
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):

4.17* (extrapolated-regression of tabulated data, temp range 76.5–246°C, Stull 1947)
4.00 (20–25°C, extrapolated, Jordan 1954)
4.12 (extrapolated liquid, Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 14092.8/(T/K)] + 8.82338; temp range 76.5–246°C (Antoine eq., Weast 1972–73)
3.83 (supercooled liquid, GC-RT correlation, Hamilton 1980)
1.12 (gas saturation, Politzki et al. 1982)
1.30 (20°C, Schmidt-Bleek et al. 1982)
1.60 (extrapolated, Mabey et al. 1982)
2.67 (Leuenberger et al. 1985)
3.26 (capillary GC-RT correlation, supercooled liquid Pt, Bidleman & Renberg 1985)
4.28 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (Pt/kPa) = 7.67323 – 2876.7/(–11.682 + T/K), temp range 349–519 K (Antoine eq., Stephenson & Malanowski 1987)
0.827 (GC-RT correlation, solid phase, Yoshida et al. 1987)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
0.405 (calculated-P/C, Mabey et al. 1982)
0.132 (8°C, calculated-P/C, Leuenberger et al. 1985)
0.523/(1 + 109.6 + 0.06) (20°C, calculated-P/C, Yoshida et al. 1987)
0.5687 (calculated-P/C, Shiu et al. 1994)
0.428 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

Octanol/Water Partition Coefficient, log Kow:
3.06 (Leo et al. 1971)
3.69 (Leo et al. 1971)
3.69, 3.62, 4.02 (Hansch & Leo 1979)
3.76 (HPLC-RT correlation, Butte et al. 1981)
3.48 (RP-HPLC-k' correlation, Miyake & Terada 1982)
4.03 (shake flask-GC, Saarikoski & Viluksele 1982)
3.72 (shake flask-HPLC/UV, Schellenberg et al. 1984)
2.97, 2.80 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
3.75, 3.69 (shake flask-GC, HPLC-k' correlation, Xie et al. 1984)
3.72 (OECD 1981 guidelines, Leuenberger et al. 1985)
3.29 (RP-HPLC-RT correlation, Chin et al. 1986)
3.97 (CPC-RV, Terada et al. 1987)
3.75 (HPLC-RT correlation, Shigeoka et al. 1988)
3.68 (batch equilibration-UV, Beltrame et al. 1988)
3.96; 3.60 (shake flask; HPLC-RT correlation, Wang et al. 1989)
3.69 (recommended, Sangster 1993)
2.67 (shake flask-GC, Kishino & Kobayashi 1994)
3.69 (recommended, Hansch et al. 1995)
3.84, 3.76, 3.65, 3.54 (pH 3.0, 6.1, 7.0, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase) measured range pH 2.1 to 13.3, Nowosielski & Fein 1998)

Bioconcentration Factor, log BCF:
2.00–2.32 (Landner et al. 1977; Laake 1982)
2.40 (fish, Köorte et al. 1978)
1.60, 1.71, 2.49 (activated sludge, algae, golden orfe, Freitag et al. 1982)
1.71; 1.81 (algae: expn; calculated, Geyer et al. 1981)
1.54–1.78, 1.60 (mussel mytilus edulis, Geyer et al. 1982)
2.92 (microorganisms-water, calculated-Kow, Mabey et al. 1982)
3.24, 3.48, 3.1–4.09 (algae, snail, guppy, Virtanen & Hattula 1982)
1.71, 2.49, 1.60 (algae, fish, activated sludge, Klein et al. 1984)
1.71, 2.13 (algae: exptl., calculated-K<sub>OW</sub>, Geyer et al. 1984)
1.78, 1.70, 2.49 (activated sludge, algae, golden ide, Freitag et al. 1985)
1.48–2.08 (rainbow trout, Oikari et al. 1985)
1.30, 2.83 (Atlantic salmon fry: humic water; lake water, Carlberg et al. 1986)
1.87–2.16 (estimated, NCASI 1992)
1.48–2.08, 3.01–4.09, 2.49, 3.48, 1.60, 1.70–3.24 (trout, guppy, fish, snail, mussel, algae, quoted from literature, NCASI 1992)
3.6, 5.4, 5.0 (perch bile to water, Söderström et al. 1994)
2.84 (Salmo salar, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K<sub>OC</sub>:

- 2.34 (sediment, Virtanen & Hattula 1982)
- 2.52 (soil, Seip et al. 1986)
- 3.41–3.84 (soil, calculated-K<sub>OW</sub>, model of Karickhoff et al. 1979, Sabljic 1987a,b)
- 3.33–3.57 (soil, calculated-K<sub>OW</sub>, model of Kenaga & Goring 1980, Sabljic 1987a,b)
- 2.52–2.75 (soil, calculated-K<sub>OW</sub>, model of Briggs 1981, Sabljic 1987a,b)
- 3.30–3.73 (soil, calculated-K<sub>OW</sub>, model of Means et al. 1982, Sabljic 1987a,b)
- 2.48–2.87 (soil, calculated-K<sub>OW</sub>, model of Chiou et al. 1983, Sabljic 1987a,b)
- 3.02 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
- 3.03 (sediment, Leuenberger et al. 1985)
- 2.99 (soil, calculated, Sabljic 1987a,b)

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>1/2</sub>:

Volatile: volatilization and sorption t<sub>1/2</sub> ~ 192 h from natural pond (Schauerte et al. 1982);
volatilization rate constant from water k = 3.90 × 10<sup>–3</sup>/(1 + 10<sup>pH–6.06</sup>)/L<sub>w</sub> h<sup>–1</sup>, L<sub>w</sub>, depth of water phase (Yoshida et al. 1987).

Photolysis: aqueous photolysis t<sub>1/2</sub> = 2–96 h, based on laboratory photolysis rate constants for an environmental pond at noon under fall sunlight conditions at 40°N latitude (Sugiura et al. 1984; quoted, Howard et al. 1991); photodegradation rate constants k<sub>p</sub> = (0.156 + 9.16 × 10<sup>4H–5.86</sup>)/(1 + 10<sup>4H–5.86</sup>)<sup>–1</sup> in water, for summer, fine day, and k<sub>p</sub> = (0.042 + 1.40 × 10<sup>4H–6.09</sup>)/(1 + 10<sup>4H–6.09</sup>) h<sup>–1</sup> in water, for winter, fine day; k = 0.72 d<sup>–1</sup> for river, k = 2.2 d<sup>–1</sup> for oligotrophic lake and k = 0.776 d<sup>–1</sup> for eutrophic lake (Yoshida et al. 1987); photochemical-transformation t<sub>1/2</sub> = 1.2 h in Xenotest 1200 (Svenson & Björndal 1988);
photoysis t<sub>1/2</sub><sub>p</sub> = 24 h (Paasivirta 1992);
photo-degradation rate constant k = 26 × 10<sup>3</sup> min<sup>–1</sup> with t<sub>1/2</sub><sub>p</sub> = 25.2 min for direct UV radiation aqueous solutions (Benitez et al. 2000).

Oxidation: aqueous oxidation rate constant k < 7 × 10<sup>4</sup> M<sup>–1</sup> h<sup>–1</sup> for singlet oxygen and k =1 × 10<sup>6</sup> M<sup>–1</sup> h<sup>–1</sup> for peroxy radical at 25°C (Mabey et al. 1982);
apparent reaction rate constant k > 10<sup>8</sup> M<sup>–1</sup> s<sup>–1</sup> at pH 8, and rate constants k <10<sup>4</sup> M<sup>–1</sup> s<sup>–1</sup> for non-protonated species, k > 10<sup>4</sup> M<sup>–1</sup> s<sup>–1</sup> for phenolate ions for the reaction with ozone in water using 3 mM t-BuOH as scavenger at pH 1.3–1.5 and 20–23°C (Hoigné & Bader 1983b).
Phenolic Compounds 2913

photooxidation $t_\text{v} = 123.4$–$1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991); photooxidation $t_\text{v} = 20.3$–$2027$ h, based on measured rate data for reaction with singlet oxygen in aqueous solution (Scully & Hoigné 1987; quoted, Howard et al. 1991);

rate constants: $k = 2 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 4.2, $k = 6 \times 10^6$ M$^{-1}$ s$^{-1}$ at pH 4.8, $k = 1.5 \times 10^7$ M$^{-1}$ s$^{-1}$ at pH 5.2, $k = 2.6 \times 10^7$ M$^{-1}$ s$^{-1}$ at pH 5.5, $k = 5.5 \times 10^7$ M$^{-1}$ s$^{-1}$ at pH 6.0, $k = 9.50 \times 10^7$ M$^{-1}$ s$^{-1}$ at pH 7 and $k = 1.2 \times 10^8$ M$^{-1}$ s$^{-1}$ at pH 9 for the reaction with singlet oxygen in aqueous solution at $(19 \pm 2)\degree\text{C}$ (Scully & Hoigné 1987);

time constant $k = (1.7 \pm 0.7) \times 10^7$ M$^{-1}$ s$^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1\degree\text{C}$ (Tratnyek & Hoigné 1991);

Biodegradation: $t_\text{v} = 7$–$10$ d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964); decompositions in soil suspensions: 5 d for complete disappearance (Woodcock 1971; quoted, Verschuuren 1983); $t_\text{s} = 216$–$432$ h and 624–1560 h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981); aqueous aerobic $t_\text{s} = 168$–$1680$ h, based on unacclimated aerobic river die-away test and soil grab sample data (Blades-Fillmore et al. 1982; Haider et al. 1974; quoted, Howard et al. 1991); aqueous anaerobic $t_\text{s} = 4050$–$43690$ h, based on unacclimated anaerobic grab sample data for soil (Baker & Mayfield 1980; quoted, Howard et al. 1991); 92% aerobic biodegraded after 28 d by both Sturm of OECD and sealed vessel tests (Birch & Fletcher 1991); biodegradation rate constant $k = 3.5 \times 10^{-11}$ L cell$^{-1}$·h$^{-1}$ at $20\degree\text{C}$ and pH 7; biodegradation rate constants $k = 8.4 \times 10^{-3}$ d$^{-1}$ in river, $k = 8.2 \times 10^{-6}$ d$^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-4}$ d$^{-1}$ in eutrophic lake in water compartment, $k = 8.4 \times 10^{-4}$ d$^{-1}$ in river, $k = 8.2 \times 10^{-5}$ d$^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-3}$ d$^{-1}$ in eutrophic lake in soil compartment (Yoshida et al. 1987); 94% reduction in concn (2-M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991) up to 60% can be mineralized by acclimated bacteria * pseudomonas aeruginosa* in 48 h but decreased with increasing humic acid concentration (Robinson & Novak 1994); Degradation constant $k = 3.2$-M/h for anaerobic batch experiment in serum bottles; $k = 2.4$ -M/h for dechlorination in anaerobic batch or continuous bioreactor; $k = 2.4$ -M/h in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999); Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^9$ mL cell$^{-1}$·h$^{-1}$ in water (Mabey et al. 1982). 

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

$k_1 = 421$ d$^{-1}$, $3573$ d$^{-1}$ (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 4.78$ d$^{-1}$, $5.26$ d$^{-1}$ (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_3 = 4.78$ d$^{-1}$, $2.54$ d$^{-1}$ (fish: bioconcentration based; toxicity based, Smith et al. 1990)

Half-Lives in the Environment:

Air: $t_\text{v} = 123.4$–$1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be $>5$ d (Kelly et al. 1994).

Surface water: $t_\text{s} = 216$–$432$ h and 624–1560 h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981); $t_\text{s} = 1.2$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988); $t_\text{s} = 2$–$96$ h, based on aqueous photolysis half-life (Sugiura et al. 1984; quoted, Howard et al. 1991); $t_\text{s} = 62$ h for the reaction with singlet oxygen at pH 8 and $(19 \pm 2)\degree\text{C}$ in water (Scully & Hoigné 1987) photolysis $t_\text{s} = 24$ h (Paasivirta 1992); photo-oxidation $t_\text{s} = 5.1$ min for reaction with Fenton’s reagent; $t_\text{s} = 20.6$ min at pH 2 and $t_\text{s} = 3.1$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).
Ground water: $t_{1/2} = 336$–43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 5 d in Dunkirk silt loam, 13 d in Mardin silt loam (Alexander & Aleem 1961)

$\tau_{\text{b}} = 168$–1680 h, based on estimated unacclimated aqueous aerobic biodegradation half-life including soil grab sample data (Haider et al. 1974; quoted, Howard et al. 1991);

$\tau_{\text{b}} = 6.3$ d in an acidic clay soil with < 1.0% organic matter and $\tau_{\text{b}} = 5.3$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch laboratory microcosm experiments (Loehr & Matthews 1992);

$\tau_{\text{b}} = 6720$ h (Paasivirta 1992).

Biota: $\tau_{\text{b}} = 0.15$ d of clearance from whole flagfish; $\tau_{\text{b}} = 0.13$ d of clearance from flagfish lipid (Smith et al. 1990).

### Table 14.1.2.9.1

Reported aqueous solubilities and vapor pressures of 2,4,6-trichlorophenol at various temperatures

<table>
<thead>
<tr>
<th>Temperature/°C</th>
<th>Aqueous solubility T/K S/kg·m⁻³</th>
<th>Vapor pressure summary of literature data t/°C P/Pa</th>
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<tr>
<td>19.5</td>
<td>410</td>
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<td>20.1</td>
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<td>24.9</td>
<td>692</td>
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</tr>
<tr>
<td>30.0</td>
<td>928</td>
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</tbody>
</table>

**Aqueous solubility**

- **Shake flask-conductivity**
  - Achard et al. 1996
  - Jaoui et al. 1999
  - Jaoui et al. 2002

- **Shake flask-optical method**
  - Jaoui et al. 1999
  - Jaoui et al. 2002

- **Shake flask-optical method**
  - Achard et al. 1996
  - Jaoui et al. 1999

<table>
<thead>
<tr>
<th>Temperature/°C</th>
<th>Aqueous solubility T/K S/kg·m⁻³</th>
<th>Vapor pressure summary of literature data t/°C P/Pa</th>
</tr>
</thead>
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<tr>
<td>76.5</td>
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<tr>
<td>105.9</td>
<td>666.6</td>
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<tr>
<td>246.0</td>
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</tbody>
</table>

**Vapor pressure**

- Stull 1947

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FIGURE 14.1.2.9.1  Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4,6-trichlorophenol.

FIGURE 14.1.2.9.2  Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorophenol.
14.1.2.10 2,3,4,5-Tetrachlorophenol

Common Name: 2,3,4,5-Tetrachlorophenol
Synonym:
Chemical Name: 2,3,4,5-tetrachlorophenol
CAS Registry No: 4901-51-3
Molecular Formula: C₆HCl₄OH
Molecular Weight: 231.891
Melting Point (°C):
116.5 (Lide 2003)
Boiling Point (°C):
   sublimation (Weast 1982–83; Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
   6.96 (Doedens 1967)
   5.30 (Sillén & Martell 1971; Kaiser et al. 1984)
   5.64 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Dean 1985; Renner 1990)
   6.35 (Schellenberg et al. 1984)
   6.61 (Xie & Dyrssen 1984)
   6.12 (Nendza & Seydel 1988)
   6.48 (Sangster 1993)
Molar Volume (cm³/mol):
   187.0 (calculated-Le Bas method at normal boiling point)
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: 0.127 (mp at 116.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
   166 (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol):
   0.140 (calculated-P/C, Shiu et al. 1994)
Octanol/Water Partition Coefficient, log Kₐw:
   4.95 (Hansch & Leo 1979)
   5.03 (HPLC-RT correlation, Banerjee et al. 1984)
   4.21 (shake flask-UV, Beltrame et al. 1984)
   4.87 (20°C, shake flask-HPLC, Schellenberg et al. 1984)
   4.82, 4.68 (shake flask-GC, HPLC-k’ correlation, Xie et al. 1984)
   4.71 (shake flask-GC, Xie & Dyrssen 1984)
   4.54 (batch equilibration-UV, Beltrame et al. 1988)
   4.21 (recommended, Sangster 1993)
   4.21 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₐa:

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Bioconcentration Factor, log BCF:
1.61, 1.60 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
2.55, 2.33 (earthworm *L. rubellus*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
2.61, 3.49, 3.53 (earthworm system, collated from literature, Connell & Markwell 1990)
0.40, 0.50, 2.30, 4.10 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC}:
4.21–4.66 (soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.77–4.01 (soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.94–3.17 (soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987a,b)
4.11–4.55 (soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987a,b)
3.20–3.60 (soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987a,b)
4.12 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
3.32 (soil, calculated-MCI χ, Sabljic 1987a,b)

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

Volatilization:
Photolysis: photochemical transformation t_{1/2} = 0.88 h in Xenotest 1200 (Svenson & Björndal 1988).
Oxidation:
Hydrolysis:
Biodegradation: 100% reduction in concn (2 µM) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)
Biotransformation: degradation rate constant k = 7.14 × 10^{-22} (± 41% SD) mol·cell^{-1}·h^{-1} from pure culture studies and k = 5 × 10^{-16} mol·cell^{-1}·h^{-1} with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

Half-Lives in the Environment:

Air:
Surface water: t_{1/2} = 0.88 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).
Ground water:
Sediment:
Soil: disappearance t_{1/2} = 43.4 d from Kooyenburg soil, t_{1/2} = 29.1 d from Holten soil with earthworm *E. fetida andrei* and t_{1/2} = 26.8 d from Kooyenburg soil, t_{1/2} = 42.5 d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988).

Biota:
14.1.2.11 2,3,4,6-Tetrachlorophenol

![Chemical Structure of 2,3,4,6-Tetrachlorophenol](image)

Common Name: 2,3,4,6-Tetrachlorophenol  
Synonym:  
Chemical Name: 2,3,4,6-tetrachlorophenol  
CAS Registry No: 58-90-3  
Molecular Formula: C₆HCl₄OH  
Molecular Weight: 231.891  
Melting Point (°C):  
70.0 (Weast 1982–83; Lide 2003)  
Boiling Point (°C):  
150 (at 15 mm Hg, Weast 1982–83)  
Density (g/cm³):  
1.60 (at 60°C, Verschueren 1983)  
Acid Dissociation Constant, pKₐ:  
5.40 (Blackman et al. 1955; Xie 1983; Schellenberg et al. 1984; Sangster 1993)  
5.46 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)  
5.30 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)  
5.22 (Uglard et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)  
5.62 (Xie & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)  
Molar Volume (cm³/mol):  
187.0 (calculated-Le Bas method at normal boiling point)  
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: 0.362 (mp at 70°C)  
Water Solubility (g/m³ or mg/L at 25°C):  
183 (shake flask-UV at pH 5.1, Blackman et al. 1955)  
180 (recommended at pH 5.1, IUPAC Solubility Data Series, Horvath & Getzen 1985)  
166 (shake flask-HPLC/UV, pH 4.62, Huang et al. 2000)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
0.763 (extrapolated-regression of tabulated data, temp range 100–275°C, Stull 1947)  
0.750 (extrapolated liquid, Antoine eq., Weast 1972–73)  
log (P/mmHg) = [–0.2185 × 15362.7/(T/K)] + 9.016052; temp range 100–275°C (Antoine eq., Weast 1972–73)  
0.692 (supercooled liq. value, GC-RT correlation, Hamilton 1980)  
0.564 (capillary GC-RT correlation, Bidleman & Renberg 1985)  
0.810 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P/Pa) = 7.96172 – 3227.92/(–6.121 + T/K); temp range 373–548 K (Antoine eq., Stephenson & Malanowski 1987)  
Henry’s Law Constant (Pa m³/mol):  
0.3548 (calculated-P/C, Shiu et al. 1994)  
Octanol/Water Partition Coefficient, log Kₖₐₖₜ:  
4.10 (Hansch & Leo 1979)  
4.27 (RP-HPLC-k’ correlation, Miyake & Terada 1982)  
4.45 (shake flask-GC, Saarikoski & Viluksela 1982)
Phenolic Compounds

4.12 (shake flask-UV, Beltrame et al. 1984)
4.42 (shake flask-HPLC/UV, Schellenberg et al. 1984)
4.42, 4.34 (shake flask-GC, HPLC-k′ correlation, Xie et al. 1984)
4.31 (shake flask-GC, Xie & Dyrssen 1984)
4.25 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
4.42 (shake flask, Shigeoka et al. 1988)
4.37 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
4.45 (recommended, Sangster 1993)
4.24 (shake flask-GC, Kishino & Kobayashi 1994)
4.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.65 (trout, Hattula et al. 1981)
2.55–2.69 (estimated, NCASI 1992)
3.3, 3.8, 4.4, 4.5 (perch bile to water, Söderström et al. 1994)

Sorption Partition Coefficient, log K<sub>OC</sub>:

4.21 (soil, calculated-K<sub>OW</sub>, model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.77 (soil, calculated-K<sub>OW</sub>, model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.94 (soil, calculated-K<sub>OW</sub>, model of Briggs 1981, Sabljic 1987a,b)
4.11 (soil, calculated-K<sub>OW</sub>, model of Means et al. 1982, Sabljic 1987a,b)
3.20 (soil, calculated-K<sub>OW</sub>, model of Chiou et al. 1983, Sabljic 1987a,b)
3.82 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
3.35 (soil, Seip et al. 1986; quoted, Sabljic 1987a,b)
3.32 (soil, calculated-MCI χ, Sabljic 1987a,b)
3.90 (calculated, Lagas 1988)
2.45, 2.70 (totally dissociated as phenolate-calculated, Lagas 1988)
3.35 (soil, calculated-MCI χ, Sabljic et al. 1995)
3.02 (2.35–3.69), 3.06 (2.31–3.81), 3.75(3.69–3.81), 2.28(2.16–2.40) (soils: organic carbon OC ≥ 0.1% and pH 3.4–7.5, OC ≥ 0.5%, OC ≥ 0.5% pH ≤ 3.4 undissociated, OC ≥ 0.5% pH ≥ 7.4 dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>½</sub>:

Volatileization:

Photolysis: aqueous photolysis t<sub>½</sub> ~ 1–336 h, based on aqueous data for 24,5−2,4,6-trichlorophenols and pentachlorophenol (Howard et al. 1991);
photo-degradation rate constant k = 21 × 10<sup>3</sup> min<sup>−1</sup> with t<sub>½</sub> = 30.6 min for direct UV radiation aqueous solutions (Benitez et al. 2000).

Photooxidation: atmospheric t<sub>½</sub> = 364.4−3644 h, based on estimated rate constant for reaction with OH radical and aqueous t<sub>½</sub> = 66.0–3480 h, based on reaction rate constants with OH and RO<sub>2</sub>· radicals with phenol class (Howard et al. 1991);
photo-oxidation rate constant k = 9 × 10<sup>3</sup> min<sup>−1</sup> with t<sub>½</sub> = 49.5 min for reaction with Fenton’s reagent; and k = 94 × 10<sup>3</sup> min<sup>−1</sup> with t<sub>½</sub> = 10.6 min at pH 2 and k = 415 × 10<sup>3</sup> min<sup>−1</sup> with t<sub>½</sub> = 1.9 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: decomposition in soil suspensions: t<sub>½</sub> > 72 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983);
aqueous aerobic t<sub>½</sub> = 672–4032 h, based on acclimated aerobic screening test data and aqueous anaerobic t<sub>½</sub> = 2688–16128 h, based on unacclimated aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:
Half-Lives in the Environment:

Air: $t_{1/2} = 364.4$–3644 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.88$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
$1–336 h$, based on estimated aqueous photolysis data for trichlorophenols and PCP (Howard et al. 1991);
photo-oxidation $t_{1/2} = 49.5$ min for reaction with Fenton’s reagent; $t_{1/2} = 10.6$ min at pH 2, and $t_{1/2} = 1.9$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

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

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + 2 d in Dunkirk silt loam (Alexander & Aleem 1961)
$672$–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
14.1.2.12 2,3,5,6-Tetrachlorophenol

Common Name: 2,3,5,6-Tetrachlorophenol
Synonym:
Chemical Name: 2,3,5,6-tetrachlorophenol
CAS Registry No: 935-95-5
Molecular Formula: C₆H₂Cl₄O, C₆HCl₄OH
Molecular Weight: 231.891
Melting Point (°C):
   115  (Weast 1982–83; Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
   5.30  (Sillen & Martell 1971)
   5.03  (Konemann 1981; Ugland et al. 1981)
   5.40  (Sangster 1993)
Molar Volume (cm³/mol):
   187.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.131 (mp at 115°C)
Water Solubility (g/m³ or mg/L at 25°C):
   100  (shake flask-HPLC/UV, pH 5.0, Ma et al. 1993)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{OW}:
   4.90  (Hansch & Leo 1979)
   4.42  (calculated-fragment constant, Konemann 1981)
   4.88  (HPLC-RT correlation, Butte et al. 1981)
   3.88  (shake flask-UV, Beltrame et al. 1984)
   4.47  (HPLC-RT correlation, Xie et al. 1984)
   3.88  (recommended, Sangster 1993)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_b:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, and Half-Lives, t½, or Lifetimes, τ:
   Biodegradation: 100% reduction in concn (2 μM) after incubation with cells of Rhodococcus chlorophenolicus for 14 d under aerobic conditions (Neilson et al. 1991)
   Biotransformation:
   Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):
Half-Lives in the Environment:
14.1.2.13 Pentachlorophenol

Common Name: Pentachlorophenol
Synonym: chlorophen, PCP, penchlorol
Chemical Name: pentachlorophenol
CAS Registry No: 87-86-5
Molecular Formula: C₆Cl₅OH
Molecular Weight: 266.336
Melting Point (°C):
191.0 (Firestone 1977; Weast 198–83)
174 (Lide 2003)
Boiling Point (°C):
309–310 (dec., Weast 1982–83)
310 (dec., Lide 2003)
Density (g/cm³):
1.987 (Firestone 1977)
1.978 (22°C, Weast 1982–83)
Acid Dissociation Constant, pKₐ:
4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)
5.00 (Farquharson et al. 1958; Renner 1990)
4.74 (Drahonovsky & Vacek 1971)
4.71 (spectrophotometric, Cessna & Grover 1978)
5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)
5.25 (Schellenberg et al. 1984)
4.90 (Xie & Dyrsen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)
4.60 (Nendza & Seydel 1988)
Molar Volume (cm³/mol):
207.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₜₐ₅ (kJ/mol):
17.5 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₜₐ₅ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₐ₅ = 56 J/mol K), F: 0.0350 (mp at 174°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):
15.4* (gravimetric method, measured range 0–70°C, Carswell & Nason 1938)
18.0 (27°C, gravimetric method, Carswell & Nason 1938)
9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)
14.0 (20°C, shake flask-UV, at pH 3.0, Bevenue & Beckman 1967)
10.0 (shake flask-gravimetric, at pH 5.0, Toyota & Kuwahara 1967)
14.0 (gravimetric at pH 5.0, Toyota & Kuwahara 1967)
5–10 (at pH 5–6 in contaminated water, Goerlitz et al. 1985)
14.0 (IUPAC recommended at pH 4.5–5.5, Horvath & Getzen 1985)
8.0 ± 2 (shake flask-UV at pH 2.5, Valsaraj et al. 1991)
32 ± 3 (shake flask-UV at pH 5.0, Valsaraj et al. 1991)
18.4 (shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)
5.0 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 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):

- 0.0227* (20°C, extrapolated-static method, measured range 100–220°C, Carswell & Nason 1938)
- 2666* (192.2°C, summary of literature data, temp range 192.2–309.3°C, Stull 1947)
- 0.108* (46.0°C, ebulliometry, measured range 46.0–233.87°C, McDonald et al. 1959)
- 0.0147–0.0227 (20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
- 0.0147 (20°C, Bevenue & Beckman 1967)
- 0.100 (extrapolated-Antoine eq., Weast 1972–73)

\[
\log (P/mmHg) = \left[ -0.2185 \times 16742.6/(T/K) \right] + 9.150200; \text{ temp range 192.2–309.3}^\circ\text{C (Antoine eq., Weast 1972–73)}
\]

- 0.231 (supercooled liq. extrapolated-Antoine eq., Weast 1976–77; quoted, Bidleman & Renberg 1985)
- 0.0213 (Firestone 1977)
- 0.0956 (supercooled liquid, GC-RT correlation, Hamilton 1980)
- 0.00415 (23°C, OECD, Klöpffer et al. 1982)
- 0.1153 (extrapolated-Antoine eq., Boublik et al. 1984)

\[
\log (P/kPa) = 7.22246 – 2846.009/(230.158 + t/°C), \text{ temp range 200–253}^\circ\text{C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

- 0.115 (capillary GC-RT, supercooled liquid P_L, Bidleman & Renberg 1985)
- 0.127 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P_{L}/kPa) = 8.198 – 3606/(T/K), \text{ temp range 463–507 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

- 0.0070* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
- 0.0147 (Howard 1991)

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

- 0.284 (calculated-P/C, Mabey et al. 1982)
- 0.0025 (calculated-P/C, Hellmann 1987)
- 0.0127 (estimated-bond contribution, Hellmann 1987)
- 0.277 (calculated-P/C, Howard 1991)
- 0.079 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

- 5.01 (Leo et al. 1971)
- 3.81 (Lu & Metcalf 1975)
- 5.01, 5.12, 5.86, 3.81 (lit. values, Hansch & Leo 1979)
- 5.01 (HPLC-RT correlation, Véith et al. 1979b)
- 5.10 (HPLC-k correlation, Butte et al. 1981)
- 4.00 (at pH 4, Renberg 1981)
- 5.08 (RP-HPLC-k correlation, Miyake & Terada 1982)
- 5.15 (shake flask-GC, Saarikoski & Vilukseta 1982; Saarikoski et al. 1986)
- 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, Harnish et al. 1983)
- 5.11 ± 0.07 (HPLC-retention volume correlation-ALPM, Garst & Wilson 1984)
- 5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 5.04, 5.08 (shake flask-GC, HPLC-k', Xie et al. 1984)
- 5.12 (Hansch & Leo 1985)
- 4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
- 2.50 (at pH 4.7, Geyer et al. 1987)
- 4.47 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
- 5.04 (HPLC-RT correlation, Shigeoka et al. 1988)
Bioconcentration Factor, log BCF:

3.75 (fish, Statham et al. 1976)
3.04 (fish, Körte et al. 1978)
2.89 (fathead minnow, Veith et al. 1979)
2.89 (fathead minnow, calculated value, Veith et al. 1979b)
3.09, 2.64 (algae: exp., 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*, Geyer et al. 1982)
3.69 (calculated-K_{OW}, Mackay 1982)
4.20 (microorganisms-water, calculated-K_{OW}, Mabey et al. 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 (*algae Chlorella fusca* in culture flasks, Geyer et al. 1984; quoted, Brockway et al. 1984)
3.10, 2.72 (algae: exp., calculated-K_{OW}, 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; quoted, Devillers et al. 1996)
0.46 (15°C, initial concn. 1.0 mg/L uptake by *allolobophora caliginosa* at 24 h, 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*, 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)
2.89 (quoted, Isnard & Lambert 1988)
2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
−2.66 (daily intake/cow adipose tissue, Travis & Arms 1988; quoted, Hattemer-Frey & Travis 1989)
4.38, 4.50, 4.53, 4.90 (earthworm system, collated from literature, Connell & Markwell 1990)
4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
2.97, 2.11 (*p. hoyi, 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)
3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)
2.33; 2.58; 2.89; 2.99; 3.23 (quoted: *Jordanella floridae; Oryzias latipes; Pimephales promelas, Brachydanio rerio; Oryzias latipes*, Devillers et al. 1996)
3.10 (*algae Chlorella fusca*, wet wt basis, Wang et al. 1996)
1.41–1.59, 1.58, 2.01–2.28 (eggshell, yolk sac, embryo of lake salmon *Salmo salar m. sebago*, calculated-C_{p}/C_{w}, Mäenpää et al. 2004)

Sorption Partition Coefficient, log K_{OC}:

2.95 (soil, calculated-K_{p}, Kenaga & Goring 1980)
4.72 (sediment-water, calculated-K_{p}, Mabey et al. 1982)
Phenolic Compounds

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; quoted, Baker et al. 2000)
3.73 (quoted average of Kenaga & Goring 1980 & 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', mobile phase buffered to pH 3, Hodson & Williams 1988)
4.40 (calculated, Lagas 1988)
3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
5.27, 5.52 (Bluepoint soil at pH 7.8, pH 7.4, 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)
4.51, 4.54 (neutral form, silt-clay slurries, Jafvert & Weber 1991)
3.06 (calculated-K_{OW}, Kollig 1993)
3.73 (soil, calculated-MCI \chi, Sabljic et al. 1995)
2.67; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
3.67, 3.45 (pH 5, 6.5, humic acid from sediments of River Arno, De Paolis & Kukkonen 1997)
3.64, 3.02 (pH 5, 6.5, HA + FA extracted from sediments of River Arno, De Paolis & Kukkonen 1997)
3.90, 3.53, 3.29 (pH 5, 6.5, 8, HA extracted from sediments of Tyrrenhian Sea, De Paolis & Kukkonen 1997)
3.51, 3.26 (pH 5, 6.5, 8, HA + FA from sediments of Tyrrenhian Sea, De Paolis & Kukkonen 1997)
3.15 (pH 5, HA extracted from water of River Arno, De Paolis & Kukkonen 1997)
3.40 (pH 5, HA + FA extracted from water of River Arno, De Paolis & Kukkonen 1997)
3.28, 3.28, 3.15 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, and pH 2.0- > 10, average, Delle Site 2001)
3.38, 3.51, 2.92 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, and pH 3.4–6.9, average, Delle Site 2001)
4.48, 4.54, 4.38 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, and pH \geq 3 undisassociated, average, Delle Site 2001)
2.82, 2.89, 2.63 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, and pH \leq 7.1 dissociated, average, Delle Site 2001)

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

Volatilization/evaporation: t_{1/2} = 84 h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);
stripping loss rate constant k = 0.0076 d^{-1} (Moos et al. 1983); k = 0.028 d^{-1} for nondissociated PCP, assuming diffusion coefficient in air to be \(7 \times 10^{-6} \text{ m}^2/\text{s}\) and in water \(7 \times 10^{-10} \text{ m}^2/\text{s}\) 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);
k(calc) = 5 \times 10^{-4} d^{-1} to 1 \times 10^{-7} d^{-1} for total PCP (Crossland & Wolff 1985).

Photolysis: photolysis: t_{1/2(calc)} = 4.75 h from observed 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/cm² 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 d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
photolysis 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_{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_{1/2} = 1.5 to 3.0 d (Crossland & Wolff 1985);
photo-transformation rate constants k = 0.6 h^{-1} with t_{1/2} = 1 h for distilled water in summer (mean temperature 25°C) and k = 0.37 h^{-1} with t_{1/2} = 2 h in winter (mean temperature 11°C); k = 0.37 h^{-1} with t_{1/2} = 2 h for
both poisoned estuarine water and estuarine water in summer and $k = 0.27 \text{ h}^{-1}$ with $t_{1/2} = 3 \text{ h}$ in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

photo-mineralization rate constants $k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for distilled water in summer (mean temperature 25°C) and $k = 0.049 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter (mean temperature 11°C); $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for poisoned estuarine water in summer and $t_{1/2} = 0.07 \text{ h}$ 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 $k = 0.10 \text{ h}^{-1}$ with $t_{1/2} = 7 \text{ d}$ for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

photochemical transformation $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988);

aqueous $t_{1/2} = 1–110 \text{ h}$ (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991)

$\text{photodegradation} k = 0.60 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0 \text{ h}$ (summer), $k = 0.37 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 2 \text{ h}$ (winter), $0.27 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Oxidation: aqueous oxidation rate constant $k < 7 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k >> 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ with 3 mM AcOH as scavenger for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983b);

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; Giüsten et al. 1981; quoted, Howard et al. 1991);

time constant $k = 4.7 \times 10^{-13} \text{ cm}^3 \text{ molecule s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at 27 ± 1°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 radical (Bunce et al. 1991).

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

Biodegradation: first order microbial degradation rate constant $k = 7.4 \times 10^{-4} \text{ h}^{-1}$ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983);

time constant $k = 1800–2160 \text{ h}$ and 480–$\infty$ h to obtain 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hansstveit 1981);

$aerobic \ k = 0.10 \text{ d}^{-1}$ with a $t_{1/2} = 7 \text{ d}$ in unadapted Nutrient Broth and $k = 1.0 \text{ d}^{-1}$ with a $t_{1/2} = 0.7 \text{ d}$ in adapted Nutrient Broth under aerobic conditions (Mills et al. 1982);

$aqueous \ t_{1/2} = 552–4272 \text{ h}$, 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);

$\text{aerobic degradation rate constant} k = 0.0017 \text{ L} \mu\text{g}^{-1} \text{d}^{-1}$ (Moos et al. 1983);

$\text{microbial degradation negligible in darkness} (\text{Hwang et al. 1986});$

$100\% \text{ reduction in concn} (2 \mu\text{M})$ after incubation with cells of Rhodococcus chlorphenolicus for 14 d under aerobic conditions (Neilson et al. 1991)

degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).

$\text{t}_{1/2} \ (\text{aerobic}) = 23 \text{ d}, \text{t}_{1/2} \ (\text{anaerobic}) = 42 \text{ d}$ in natural waters (Capel & Larson 1995)

$\text{Biotransformation: first order fish metabolism} k = 1.5 \times 10^{-3} \text{ h}^{-1}$ (Sanborn et al. 1975, quoted, Addision et al. 1983);

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

$\text{degradation rate} k = 3 \times 10^{-14} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

$k_1 = 18.3 \text{ h}^{-1}, 19 \text{ h}^{-1}$ (at 1 mM buffer concn.), 18.5 h$^{-1}$ (at 10 mM buffer concn.) at pH 8 (guppy p. reticulata, Saarikoski et al. 1986)

$k_1 = 222 \text{ d}^{-1}, 1677 \text{ d}^{-1}$ (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}, 1.03 \text{ d}^{-1}$ (flagfish: whole fish; fish lipid, Smith et al. 1990)
\[ k_2 = 1.03 \text{ d}^{-1}, \ 0.95 \text{ d}^{-1} \text{ (flagfish: BCF based, toxicity based, Smith et al. 1990)} \]

\[ k_2 = 0.00195 \pm 0.00063 \text{ h}^{-1} \ (m. \ relicta, \ Landrum \ & \ Dupuis \ 1990) \]

\[ k_2 = 0.00330 \pm 0.00140 \text{ h}^{-1} \ (p. \ hoyi, \ Landrum \ & \ Dupuis \ 1990) \]

\[ k_1 = 662.4 \text{ d}^{-1}, k_2 = 0.502 \text{ d}^{-1} \text{ (algae Chlorella fisca, Wang et al. 1996)} \]

\[ k_1 = 0.733 \text{ d}^{-1}, k_2 = 0.020 \text{ d}^{-1} \text{ (eggs/hell of dissected parts of lake salmon, Mäenpää et al. 2004)} \]

\[ k_1 = 0.680 \text{ d}^{-1}, k_2 = 0.000 \text{ d}^{-1} \text{ (yolk sac of dissected parts of lake salmon, Mäenpää et al. 2004)} \]

\[ k_1 = 2.828 \text{ d}^{-1}, k_2 = 0.015 \text{ d}^{-1} \text{ (embryo of dissected parts of lake salmon, Mäenpää et al. 2004)} \]

Half-Lives in the Environment:

Air: tropospheric lifetime of 4 d for reaction with OH radical on March 21 at 43°N (Bunce et al. 1991);

\[ t_{1/2} = 139.2-1392 \text{ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radicals in air; photolysis } t_{1/2} = 6.5 \text{ h in noonday summer sunshine (Howard 1991); atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).} \]

Surface water: calculated photolysis \[ t_{1/2} = 4.75 \text{ h from a determined rate } k = 3.4 \times 10^{-4} \text{ s}^{-1} \text{ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm}^2 \text{ 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} \text{ for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983); estimated direct photolysis midday } t_{1/2} = 20 \text{ min from experimentally determined rate constant } k = 2.1 \text{ h}^{-1} \text{ (quoted unpublished result, Zepp et al. 1984); } 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 (summer), } t_{1/2} = 2 \text{ h (winter) for distilled water; } t_{1/2} = 2 \text{ h (summer), } t_{1/2} = 3 \text{ h (winter) for estuarine water; } t_{1/2} = 2 \text{ h (summer), } t_{1/2} = 3 \text{ h (winter) for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986); } t_{1/2} = 6 \text{ d (summer), } t_{1/2} = 14 \text{ d (winter) for distilled water; } t_{1/2} = 3 \text{ d (summer), } t_{1/2} = 7 \text{ d (winter) for estuarine water; } t_{1/2} = 6 \text{ d (summer), } t_{1/2} = 10 \text{ d (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 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björn Dahl 1988); } t_{1/2} = 1-110 \text{ h, based on aqueous photolysis half-life (Howard et al. 1991); photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991); photodegradation } t_{1/2} = 1.0 \text{ h (summer), } t_{1/2} = 2.0 \text{ h (winter) in distilled water and } t_{1/2} = 2.0 \text{ h (summer), } t_{1/2} = 3.0 \text{ h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).} \]

\[ t_{1/2} = 23 \text{ d, } t_{1/2} = 42 \text{ d in natural waters (Capel & Larson 1995)} \]

Ground water: \[ t_{1/2} = 1104-36480 \text{ h, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et al. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).} \]

Sediment: first order microbial degradation rate constant \[ k = 7.4 \times 10^{-4} \text{ h}^{-1} \text{ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983).} \]

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam (Alexander & Aleem 1961) disappearance \[ t_{1/2} = 23.2 \text{ d from Kooyenburg soil, } t_{1/2} = 47.9 \text{ d from Holten soil with earthworm e. fetida andrei and } t_{1/2} = 27.4 \text{ d from Kooyenburg soil, } t_{1/2} = 31.8 \text{ d from Holten soil with earthworm l. rubellus (van Gestel & Ma 1988); } t_{1/2} = 552-4272 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); } t_{1/2} = 2.0 \text{ d in an acidic clay soil with } < 1.0% \text{ organic matter and } t_{1/2} = 6.7 \text{ d in a slightly basic sandy loam soil with } 3.25% \text{ organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).} \]

Biota: biological \[ t_{1/2} = 30 \text{ d in guppy lebistes reticulatus(Landner et al. 1977); elimination } t_{1/2} = 23, 9.3, 6.9, \text{ and } 6.2 \text{ h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980); estimated } t_{1/2} = 7.0 \text{ d in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985); clearance from flagfish: } t_{1/2} = 0.68 \text{ d from whole fish and } t_{1/2} = 0.68 \text{ d from fish lipid (Smith et al. 1990).} \]
### TABLE 14.1.2.13.1

Reported aqueous solubilities of pentachlorophenol at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>T/K</th>
<th>S/g·m⁻³</th>
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<td>173.1</td>
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Note: PCP data in Table I incorrect, correction made

Figure 3 in ref.

Based on Figure 3 in ref.

**FIGURE 14.1.2.13.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for pentachlorophenol.
### TABLE 14.1.2.13.2
Reported vapor pressures of pentachlorophenol at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Carswell &amp; Nason 1938</th>
<th>Stull 1947</th>
<th>McDonald et al. 1959</th>
<th>Rordorf 1989</th>
</tr>
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<td>summary of literature data</td>
<td>ebulliometry</td>
<td>gas saturation-GC</td>
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<td>P/Pa</td>
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<td>192.2</td>
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<tr>
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<td>A</td>
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<tr>
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<td>B</td>
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measured range 100–220°C

*extrapolated from graph

---

**FIGURE 14.1.2.13.2** Logarithm of vapor pressure versus reciprocal temperature for pentachlorophenol.
14.1.2.14 4-Chloro-\textit{m} cresol

![Structure of 4-Chloro-\textit{m} cresol]

Common Name: 4-Chloro-\textit{m} cresol
Synonym: \textit{p}-chloro-\textit{m}-cresol, 2-chloro-5-hydroxytoluene, 4-chloro-3-methylphenol
Chemical Name: 4-chloro-\textit{m}-cresol, 4-chloro-3-methylphenol
CAS Registry No: 59-50-7
Molecular Formula: \textit{C}_7\textit{H}_7\textit{Cl}_1\textit{O}_1, \textit{CH}_3(\textit{Cl})\textit{C}_6\textit{H}_3\textit{OH}
Molecular Weight: 142.583
Melting Point (°C):
- 67 (Lide 2003)
Boiling Point (°C):
- 235.0 (Weast 1977; Callahan et al. 1979; Dean 1985; Lide 2003)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
- 146.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.387 (mp at 67°C)
Water Solubility (g/m³ or mg/L at 25°C):
- 3990 (shake flask-UV with buffer at pH 5.1, Blackman et al. 1955)
- 3990 (IUPAC selected, Horvath & Getzen 1985)
- 3650 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
Vapor Pressure (Pa at 25°C):
- 6.67 (Mabey et al. 1982)
Henry’s Law Constant (Pa m³/mol at 25°C):
- 0.253 (20°C, calculated-P/C, Mabey et al. 1982)
Octanol/Water Partition Coefficient, log K_{ow}:
- 2.18 (Hansch & Leo 1979)
- 2.95 (calculated as per Tute 1971, Callahan et al. 1979)
- 3.10 (HPLC-RT correlation, Veith et al. 1979)
- 3.10 (recommended, Sangster 1993)
- 3.10 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
- 2.60 (microorganisms-water, calculated-K_{ow}, Mabey et al. 1982)
Sorption Partition Coefficient, log K_{OC}:
- 2.78 (sediment-water, calculated-K_{ow}, Mabey et al. 1982)
Environmental Fate Rate Constants, \textit{k}, and Half-Lives, \textit{t}_{1/2}:
Oxidation: rate constants \textit{k} < 7 \times 10^5 M^{-1} h^{-1} for singlet oxygen and \textit{k} = 1 \times 10^7 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).
Biotransformation: bacterial transformation \textit{k} = 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1} in water (Mabey et al. 1982).

Half-Lives in the Environment:
14.1.3 NITROPHENOLS

14.1.3.1 2-Nitrophenol

Common Name: 2-Nitrophenol
Synonym: o-nitrophenol, 2-hydroxynitrobenzene
Chemical Name: 2-nitrophenol
CAS Registry No: 88-75-5
Molecular Formula: C₆H₅NO₂, C₆H₄(NO₂)OH
Molecular Weight: 139.109
Melting Point (°C): 44.8 (Lide 2003)
Boiling Point (°C): 216.0 (Weast 1982-83; Lide 2003)
Density (g/cm³ at 20°C):
1.485, 1.2942 (14, 40°C, Weast 1982–83)
131.9 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₘₐₜ:
7.21 (Pearce & Simkins 1968)
7.23 (Serjeant & Dempsey 1979)
8.28 (Mabey et al. 1982)
7.22 (Dean 1985)
Enthalpy of Fusion, ∆Hₜₚₚ (kJ/mol):
17.57 (Tsonopoulos & Prausnitz 1971)
17.44 (Beneš & Dohnal 1999)
Entropy of Fusion, ∆Sₜₚₚ (J/mol K):
55.23 (Tsonopoulos & Prausnitz 1971)
48.95, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ∆Sₜₚₚ = 56 J/mol K), F: 0.630 (mp at 44.8°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
3210* (38.4°C, shake flask-residue volume method, measured range 34.8–196°C, critical solution temp above 200°C, Sidgwick et al. 1915)
1390, 1095 (20°C, shake flask-UV, calculated, Hashimoto et al. 1984)
1080* (20 ± 0.5°C, shake flask-UV with buffer at pH 1.5, measured range 5–30°C, Schwarzenbach et al. 1985)
2100 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
1697* (24.8°C, shake flask-conductimetry, measured range 15.6–34.7°C, Achard et al. 1996)
1350* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)
1169* (17.35°C, shake flask-optical method, measured range 290.5–322.7 K, Jaoui et al. 2002)
ln [S/(mol kg–1)] = 16.237 − 4672.3/(T/K); temp range 288–308 K (eq. derived using reported exptl. data, Jaoui et al. 2002)
ln [S/(mol kg–1)] = 6.9022 − 1784.4/(T/K); temp range 308–332 K (eq. derived using reported exptl. data, Jaoui et al. 2002)
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):
29.10* (extrapolated-regression of tabulated data, temp range 49.3–214.5°C, Stull 1947)
log (P/mmHg) = [−0.2185 × 12497.3/(T/K)] + 8.497320; temp range 49.3–214.5°C (Antoine eq., Weast 1972–73)
24.43 (extrapolated-Cox eq., Chao et al. 1983)
\[ \log (P/\text{mmHg}) = [1 - 487.905/(T/\text{K})] \times 10^{0.885400 - 6.30106 \times 10^{-4}(T/\text{K}) + 6.42867 \times 10^{-7}(T/\text{K})^2}; \text{ temp range: 322.5–487.7 K (Cox eq., Chao et al. 1983)} \]
12.4 ± 0.2 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
17.25 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P_g/\text{kPa}) = 7.8446 - 2864.6/(101.17 + T/\text{K}), \text{ temp range 273–292 K (solid, Antoine eq.-I., Stephenson & Malanowski 1987)} \]
\[ \log (P_l/\text{kPa}) = 6.04963 - 1571.7/(T/\text{K}), \text{ temp range 366–490 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)} \]
18.86 (supercooled liquid \( P_l \) at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
10.61 (20°C, solid \( P_s \), converted from \( P_l \) with \( \Delta S_{\text{fus}} \) and mp, Schwarzenbach et al. 1988)
\[ \log (P/\text{atm}) = 5.735 - 2776/(T/\text{K}) \] (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

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):
0.766 (calculated-P/C, Mabey et al. 1982)
0.355 (Leuenberger et al. 1985)
1.367 (20°C, calculated-P/C, Schwarzenbach et al. 1988)
1.25* (gas stripping-UV, measured range 5–40°C, Müller & Heal 2001)
\[ \ln [H/(\text{M atm}^{-1})] = 6290/(T/\text{K}) - 16.6; \text{ temp range 278–303 K (gas stripping-UV, Müller & Heal 2001)} \]
1.178* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)
\[ \ln [H/(\text{M atm}^{-1})] = 6270/(T/\text{K}) - 16.6; \text{ temp range 284–302 K, Harrison et al. 2002)} \]

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
1.79 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971)
2.00 (shake flask, Uemiyama et al. 1971)
1.25, 1.18 (calculated-fragment const., calculated-\( \pi \) const., Rekker 1977)
1.79 (shake flask, Korenman et al. 1977)
1.68 (shake flask at pH 7, Unger et al. 1978)
1.35 (HPLC-RT correlation, Veith et al. 1979)
1.91 (HPLC-RT correlation, Miyake et al. 1986)
1.89 (21.5 ± 0.5°C, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
1.76 (shake flask-UV, Kramer & Henze 1990)
1.68 (CPC-RV at pH 7.4, El Tayar et al. 1991)
2.24 (HPLC-RT correlation, Saito et al. 1993)
1.77 (recommended, Sangster 1993)
1.85, 1.79 (COMPUTOX databank, Kaiser 1993)
1.79, 1.68 (recommended, value at pH 7.4; Hansch et al. 1995)
2.03 (solid-phase microextraction, Dean et al. 1996)
1.63, 1.99, 2.28, 1.90 (HPLC-k’ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, log BCF:
2.10 (bluegill sunfish, Veith et al. 1980)
1.23 (microorganisms-water, calculated-\( K_{\text{OW}} \), Mabey et al. 1982)
1.15 (calculated-\( K_{\text{OW}} \), Howard 1989)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):
1.43 (sediment-water, calculated-\( K_{\text{OW}} \), Mabey et al. 1982)
1.81 (soil, calculated-S, quoted, Howard 1989)
2.17, 2.50 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
2.043, 1.758, 1.854, 1.708, 2.283 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
Phenolic Compounds


Environmental Fate Rate Constants, k, or Half-Lives, \( t_{1/2} \):
Volatilization: volatilization \( t_{1/2} = 296 \) h from a model river was estimated using Henry’s law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989)

Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures see reference:
rate constant \( k < 2 \times 10^6 \) M⁻¹·h⁻¹ for singlet oxygen, and \( k = 2 \times 10^6 \) M⁻¹·h⁻¹ for peroxy radical at 25°C (Mabey et al. 1982);
\( k_{OH} = 0.922 \times 10^{-12} \) cm³·molecule⁻¹·s⁻¹ at 296 K (Becker et al. 1984; quoted, Cartier et al. 1986);
\( k_{OH}(\text{exptl}) = 0.92 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹, \( k_{OH}(\text{calc}) = 3.4 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)
\( k_{OH}(\text{exptl}) = 0.9 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹, \( k_{OH}(\text{calc}) = 4.4 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1987)
\( k_{OH} = 0.90 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at 294 K (Atkinson 1989)
\( k_{OH} = (2.34 \pm 0.33) \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at (24.6 ± 0.4) °C (Edney et al. 1986)
\( k_{OH} = 2.34 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at 298 K, \( k_{NO3} = 9.7 \times 10^{-17} \) cm³ molecule⁻¹ s⁻¹ at 296 K (Atkinson 1990)
\( k_{NO3} < 0.02 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at 296 K and \( k_{OH} = 0.90 \times 10^{-12} \) cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)
aqueous photooxidation \( t_{1/2} = 480 \) min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)

photo-transformation decay rate constant \( k = 0.27 \) min⁻¹ on 0.2 g/L of TiO₂ solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);
average rate of biodegradation 14.0 mg COD g⁻¹·h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978);
aqueous aerobic \( t_{1/2} = 168–672 \) h, based on unacclimated aerobic screening test data (Sasaki 1978; Gerike & Fischer 1979; selected, Howard et al. 1991);
aqueous anaerobic \( t_{1/2} = 168–672 \) h, based on anaerobic soil grab sample data (Sudhakar-Barik & Sethunathan 1978; selected, Howard et al. 1991).

Biotransformation: estimated bacterial transformation rate constant of \( 2 \times 10^{-9} \) 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: \( t_{1/2} = 14 \) h for the gas phase reaction with hydroxyl radical (GEMS 1986; quoted, Howard 1989)
photooioxidation \( t_{1/2} = 7–71 \) h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: \( t_{1/2} = 168–672 \) h, based on aerobic river die-away test data (Ludzack et al. 1958; selected value, Howard et al. 1991);
volutilization \( t_{1/2} = 12 \) d from a model river was estimated using Henry’s law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind and \( t_{1/2} = 1–8 \) d in freshwater (Howard 1989);
calculated \( t_{1/2} = 390 \) h for a body of water with 1 m in depth (Schmidt-Bleek et al. 1982; quoted, Howard 1989);
photooxidation \( t_{1/2} = 480 \) min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: \( t_{1/2} = 336–672 \) h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: \( t_{1/2} = 10 \) d in flooded soil (Howard 1989);
t_{1/2} = 168–672 h, based on estimated aqueous aerobic biodegradation half-life and anaerobic soil grab sample data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 14.1.3.1.1</th>
</tr>
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<tbody>
<tr>
<td>Reported aqueous solubilities of 2-nitrophenol at various temperatures</td>
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<td>shake flask-UV spec</td>
<td>shake flask-optical method</td>
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*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.
FIGURE 14.1.3.1.1 Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for 2-nitrophenol.

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<th>Vapor pressure</th>
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</table>

For gas-to-liquid transfer
\( \Delta H^o/(kJ mol^{-1}) = -52.3 \pm 8.1 \)
\( \Delta S^o/(J mol^{-1}K^{-1}) = -138 \pm 28 \)
FIGURE 14.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrophenol.

FIGURE 14.1.3.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for 2-nitrophenol.
14.1.3.2 3-Nitrophenol

Common Name: 3-Nitrophenol  
Synonym: m-nitrophenol  
Chemical Name: 3-nitrophenol  
CAS Registry No: 554-84-7  
Molecular Formula: C₆H₅NO₂, C₆H₄(NO₂)OH  
Molecular Weight: 139.109  
Melting Point (°C):  
96.8 (Lide 2003)  
Boiling Point (°C):  
194.0 (at 70 mm Hg, Weast 1982–83)  
Density (g/cm³ at 20°C):  
1.2797 (10°C, Verschueren 1983)  
Molar Volume (cm³/mol):  
108.7 (100°C, Stephenson & Malanowski 1987)  
131.9 (calculated-Le Bas method at normal boiling point)  
Acid Dissociation Constant, pKₐ:  
8.00 (Fieser & Fieser 1958)  
8.36 (Serjeant & Dempsey 1979; Dean 1985; Howard 1989; Haderlein & Schwarzenbach 1993)  
Enthalpy of Fusion, ΔHₚ (kJ/mol):  
21.34 (Tsonopoulos & Prausnitz 1971)  
19.20 (Beneš & Dohnal 1999)  
Entropy of Fusion, ΔSₚ (J/mol K):  
57.74 (Tsonopoulos & Prausnitz 1971)  
Fugacity Ratio at 25°C (assuming ΔSₚ = 56 J/mol K), F: 0.197 (mp at 96.8°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):  
30300* (40.4 °C, shake flask-residue volume method, measured range 40.4–98.7 °C, critical solution temp 98.7°C, Siddwick et al. 1915)  
13000 (shake flask-UV spectrophotometry, Roberts et al. 1977)  
11546 (20°C, shake flask-UV, Hashimoto et al. 1984)  
10800* (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):  
3.83 × 10⁻² (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (Pᵥ/kPa) = 8.93697 – 3981.386/(T/K), temp range 305–334 K (solid, Antoine eq., Stephenson & Malanowski 1987)  
99.98 (Weber et al. 1981)  

Henry’s Law Constant (Pa·m³/mol at 25°C):  
2.203 × 10⁻⁴ (quoted, Gaffney et al. 1987)  
1.033 (calculated-P/C, Howard 1989)  

Octanol/Water Partition Coefficient, log Kₒₒₖ:  
2.00 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)  
2.00 (shake flask-UV at pH 5.6, Umeyama et al. 1971)  
2.00 (20°C, shake flask, Korenman et al. 1976)
Bioconcentration Factor, log BCF:
1.40 (goldfish, ratio of rate constant $k_1/k_2$, Nagel & Urich 1980)
1.40 ($Brachydanio rerio$, Butte et al. 1987)
1.28 (estimated-$K_{OW}$, Howard 1989)

Sorption Partition Coefficient, log $K_{OC}$:
1.72 (Brookton clay loam, Boyd 1982)
1.36 (soil, estimated-$S$, Howard 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization: volatilization $t_{1/2} = 4.2$ d from a model river was estimated using Henry’s law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989).

Photolysis:
Oxidation: photooxidation $t_{1/2} ~ 14$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard 1989);
phototransformation decay rate $k = 0.18$ min$^{-1}$ in 0.2 g/L of TiO$_2$ solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);
decomposition by a soil microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)
complete degradation of 16 mg/L in 3–5 d by wastewater, and 3–5 d by soil (Haller 1978);
average rate of biodegradation 17.5 mg COD g$^{-1}$·h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
$t_{1/2} = 6.3$ d or less in flooded soil under anaerobic conditions (Howard 1989)
$t_{1/2}$(aerobic) = 0.76 d, t_{1/2}$(anaerobic) = 6.8 d in natural waters (Capel & Larson 1995).

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$k_1 = 1.54$ h$^{-1}; k_2 = 0.00$ h$^{-1}$ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:
Air: $t_{1/2} = 14$ h for reaction with hydroxyl radical in vapor phase (Howard 1989).
Surface water: $t_{1/2} = 4.2$ d in a model river (Howard 1989)
$t_{1/2}$(aerobic) = 0.76 d, $t_{1/2}$(anaerobic) = 6.8 d in natural waters (Capel & Larson 1995).

Groundwater:

Sediment:
Soil: $t_{1/2} = 6.3$ d in flooded soil under anaerobic conditions (Howard 1989).
Biota: elimination from goldfish within 4 h (Nagel & Urich 1980).
TABLE 14.1.3.2.1
Reported aqueous solubilities of 3-nitrophenol at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
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<td>634700</td>
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Enthalpies of solution*:
- $\Delta H_{\text{sol (solid)}} = 29.3 \text{ kJ mol}^{-1}$
- $\Delta H_{\text{sol (liq.)}} = 16.1 \text{ kJ mol}^{-1}$

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

FIGURE 14.1.3.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-nitrophenol.
14.1.3.3 4-Nitrophenol

Common Name: 4-Nitrophenol
Synonym: p-nitrophenol, 4-hydroxynitrobenzene
Chemical Name: 4-nitrophenol
CAS Registry No: 100-02-7
Molecular Formula: C₆H₅NO₂, C₆H₄(NO₂)OH
Molecular Weight: 139.109

113.6 (Lide 2003)
Boiling Point (°C): 279.0 (decomposes, Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C): 1.479 (Weast 1982–83)
Molar Volume (cm³/mol):
131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pKₐ:
7.08 (21.5°C, UV, Schwarzenbach et al. 1988)
7.17 (Fieser & Fieser 1958)
7.16 (Serjeant & Dempsey 1979; Howard 1989; Haderlein & Schwarzenbach 1993)
7.15 (Dean 1985; Miyake et al. 1987; Brecken-Folse et al. 1994; Howe et al. 1994)

Enthalpy of Fusion, ΔHfus (kJ/mol):
15.90 (Tsonopoulos & Prausnitz 1971)
18.25 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔSfus (J/mol K):
41.09 (Tsonopoulos & Prausnitz 1971)
62.76, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.135 (mp at 113.6°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):
29100* (34.8°C, shake flask-residue volume method, measured range 34.8–92.8°C, critical solution temp 92.8°C, Sidgwick et al. 1915)
14000 (shake flask-spectrophotometry, Roberts et al. 1977)
9950, 14800 (15, 25°C, shake flask, average values of 6 laboratories, OECD 1981)
13490, 11140 (20°C, shake flask-UV, calculated, Hashimoto et al. 1984)
11570 (20 ± 0.5°C, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
16000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
15599* (shake flask-conductimetry, measured range 15.3–34.9°C, Achard et al. 1996)
12200* (20°C, shake flask-UV spectrophotometry, measured range 10–38°C, Beneš & Dohnal 1999)
15052* (23.65°C, shake flask-optical method, measured range 285.9–313.8 K, Jaoui et al. 2002)

\[ \ln \left( \frac{S}{(\text{mol kg}^{-1})} \right) = 17.110 - 4273.4/(T/K); \text{ temp range 288–314 K} \] (eq. derived using reported explt. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0054 (20°C, Schmidt-Bleek et al. 1982)
0.0012 (selected, Yoshida et al. 1983)
0.0044 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P_p/\text{kPa}) = 11.9529 - 5159.7/(T/K), \text{ temp range 304–352 K} \] (solid, Antoine eq., Stephenson & Malanowski 1987)
Phenolic Compounds

0.111  (supercooled liquid $P_L$ at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
0.0131  (20°C, solid $P_S$, converted from $P_L$ with $\Delta S_{\text{fus}}$ and mp, Schwarzenbach et al. 1988)
log ($P$/mmHg) = 8.305 – 4180/(T/K) (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)
0.133  (Howard 1989)

Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
4.21 × 10$^{-5}$ (exptl., Hine & Mookerjee 1975)
5.55 × 10$^{-4}$, 9.87 × 10$^{-3}$ (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1.04 × 10$^{-5}$ (calculated-P/C, Yoshida et al. 1983)
0.00335 (20°C, calculated-P/C, Schwarzenbach et al. 1988)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
1.91  (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
1.18, 1.27  (calculated-$\pi$ const., calculated-fragment const., Rekker 1977)
1.68 ± 0.01  (RP-HPLC-$k'$ correlation, Unger et al. 1978)
2.07  (RP-HPLC-$k'$ correlation, Miyake & Terada 1982)
1.86  (HPLC-ref. substances extrapolated, Harnish et al. 1983)
1.88  (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
1.96 ± 0.08  (HPLC-RV correlation.-ALPM, Garst 1984; Garst & Wilson 1984)
0.70  (calculated-$\gamma$ from UNIFAC, Campbell & Luthy 1985)
1.90  (HPLC-RV correlation, Brooke et al. 1986)
2.10  (HPLC-$k'$ correlation, Miyake et al. 1987)
1.93  (shake flask/batch equilibration-UV, Beltrame et al. 1988, 1989)
2.04  (21.5 ± 1.5°C, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
1.77  (CPC-RV at pH 7.4, El Tayar et al. 1991)
1.85, 1.91  (COMPUTOX databank, Kaiser 1993)
1.91  (recommended, Sangster 1993)
1.90 ± 0.14, 1.09 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-$k'$ correlation, Cichna et al. 1995)
1.91  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log $BCF$:
2.10  (fathead minnow, Veith et al. 1980)
2.56  (mean whole body $^{14}$C in fathead minnow, Call et al. 1980)
1.90, 2.34  (total $^{14}$C in fathead minnow: observed, calculated, mean exposure level 0.0041 µg·mL$^{-1}$, Call et al. 1980)
2.44, 2.65  (total $^{14}$C in fathead minnow: observed, calculated, mean exposure level 0.0441 µg·mL$^{-1}$, Call et al. 1980)
1.76; 1.04  (golden orfe; green algae, Freitag et al. 1982)
1.48  (activated sludge, Freitag et al. 1982)
1.43  (microorganisms-water, calculated-$K_{\text{OW}}$, Mabey et al. 1982)
0.301  (calculated-$K_{\text{org}}$, Yoshida et al. 1983)
1.48, 1.45  (alga chlorella fusca, wet wt. basis, calculated-$K_{\text{org}}$, Geyer et al. 1984)
1.60, 1.48, 1.48  (golden ide, algae, activated sludge, Freitag et al. 1985)
1.90  (fathead minnow, quoted, Howard 1989)

Sorption Partition Coefficient, log $K_{\text{OC}}$:
1.65  (sediment-water, calculated-$K_{\text{org}}$, Mabey et al. 1982)
2.41  (soil, calculated-$K_{\text{org}}$, Yoshida et al. 1983)
1.74  (Brookston clay loam, Boyd 1982)
2.18  (HPLC-$k'$ correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
1.32  (soil, calculated-$S$, Howard 1989)
2.37  (soil, quoted exptl., Meylan et al. 1992)
2.49  (soil, calculated-MCl $\chi$ and fragment contribution, Meylan et al. 1992)
2.16, 2.07 (RP-HPLC-k’ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.05; 2.49 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
2.03, 1.94 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, and pH ≤ 5.4, average, Delle Site 2001)

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

Volatile:
Photolysis: atmospheric photolysis t½ = 3.1–329 h, based on sunlight photolysis at pH 9 and pH 4 (Hustert et al. 1981; Lemaire et al. 1985; selected, Howard et al. 1991); rate constant k = 3.96 × 10⁻³ h⁻¹ for the direct photolysis in water (Yoshida et al. 1983); photolysis t½ range from hours to a week or more in atmosphere and t½ = 2–14 d in clear surface waters (Howard 1989).

Oxidation: oxidation rate constant k < 2 × 10⁵ M⁻¹·h⁻¹ for singlet oxygen, k = 2 × 10⁶ M⁻¹·h⁻¹ for peroxy radical (Mabey et al. 1982); photooxidation t½ = 21 d to 5.6 y in water, based on rate constants for reaction in water with hydroxyl radical (Dorfman & Adams 1973; Scully & Hoigné 1987; selected, Howard et al. 1991); rate constant k < 50 M⁻¹·s⁻¹ for 0.01–14 mM to react with ozone in water using PrOH as scavenger at pH 1.7 and 20–23°C in water (Hoigné & Bader 1983a,b); rate constant k = 8.3 × 10⁻¹² cm³·molecule⁻¹·s⁻¹ for the gas-phase reaction with OH radical at 296 K in the atmosphere (Becker et al. 1984; quoted, Carlier et al. 1986); photooxidation t½ = 14.5–145 h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991); aqueous photooxidation t½ = 440 min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992); phototransformation decay k = 0.15 min⁻¹ on 0.20 g/L of TiO₂ solution (Minero et al. 1993).

Hydrolysis:
Biodegradation: 95% degradation in 3–6 d in mixture bacteria cultures (Tabak et al. 1964); decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); average rate of biodegradation 17.5 mg COD g⁻¹·h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978); aqueous aerobic t½ = 18.2–168 h, based on pond die-away test data (Paris et al. 1983; Bourquin 1984; selected, Howard et al. 1991); aqueous anaerobic t½ = 163–235 h, based on anaerobic die-away data in two different flooded soils (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991); was not biodegraded with activated sludge at a concn. of 94 mg/L but completely degraded with a decreased concn. of 19 mg/L in 28 d expt. (Kool 1984).

Biotransformation: estimated bacterial transformation rate constant of 1.00 × 10⁻⁷ mL·cell⁻¹·h⁻¹ in water (Mabey et al. 1982); rate constant of (3.80 ± 1.40) × 10⁻¹¹ L·organism⁻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 = 14.5–145 h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991); atmospheric transformation lifetime was estimated to be 1–5 to > 5 d (Kelly et al. 1994).
Surface water: photodegradation t½ = 5.7 d at pH 5, t½ = 6.7 d at pH 7 and t½ = 13.7 d at pH 9 in water (Hustert et al. 1981); t½ = 1–8 d in freshwater, t½ = 1–3 yr in marine systems but decreased to 13–20 d with the presence of sediment, the mean t½ = 7.7 d estimated by a nonsteady-state equilibrium model, and photolysis t½ = 2–14 d in clear surface waters (Howard 1989); t½ = 18.2–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); t½ = 440 min for photolysis in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).
Groundwater: \( t_{1/2} = 36.4-235 \) h, based on pond die-away test data and anaerobic die-away data in two different flooded soils (Paris et al. 1983; Sudhakar-Barik & Sethunnathan 1978; quoted, Howard et al. 1991).

Sediment:

Soil: \( t_{1/2} \approx 1 \) d in agricultural topsoil and \( t_{1/2} = 10 \) d in flooded soil, \( t_{1/2} > 40 \) d in subsoil under aerobic conditions and longer still under anaerobic conditions (Howard 1989);

\( t_{1/2} = 17-29 \) h, based on aerobic soil die-away test data (Loekke 1985; selected, Howard et al. 1998).

\( t_{1/2} = 75 \) d in a coarse sandy soil, \( t_{1/2} = 145 \) d in sandy loam (Kjeldsen et al. 1990)

Biota: depuration \( t_{1/2} \text{(obs.)} = 72 \) h, \( t_{1/2} \text{(calc)} = 37 \) h for mean exposure level of 0.0041 \( \mu g \cdot mL^{-1} \) and \( t_{1/2} \text{(obs.)} = 228 \) h, \( t_{1/2} \text{(calc)} = 206 \) h for mean exposure level of 0.041 \( \mu g \cdot mL^{-1} \) (Call et al. 1980).

### TABLE 14.1.3.3.1

**Reported aqueous solubilities of 4-nitrophenol at various temperatures**

<table>
<thead>
<tr>
<th></th>
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<td>‡mean, 13800–15900 g·m⁻³</td>
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</table>

Enthalpies of solution:

- \( \Delta H_{\text{sol}} \text{(solid)} = 28.9 \text{ kJ mol}^{-1} \)
- \( \Delta H_{\text{sol}} \text{(liq.)} = 16.9 \text{ kJ mol}^{-1} \)
- \( \Delta H_{\text{sol}} \text{(K]} = 386.95 \text{ K} \)
- \( \Delta H_{\text{sol}} \text{(solid)} = 28.9 \text{ kJ mol}^{-1} \)

Critical solution temp 92.8°C

Triple point 39.6°C

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.*
FIGURE 14.1.3.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-nitrophenol.
14.1.3.4 2,4-Dinitrophenol

Common Name: 2,4-Dinitrophenol
Synonym: 2,4-hydroxynitrobenzene, Aldifen, 2,4-DNP
Chemical Name: 2,4-dinitrophenol
CAS Registry No: 57-28-5
Molecular Formula: C₆H₄N₂O₅, C₆H₃(NO₂)₂OH
Molecular Weight: 184.106
Melting Point (°C):
114.8  (Lide 2003)
Boiling Point (°C):
sublimation  (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
1.684  (24°C, Weast 1982–83)
Molar Volume (cm³/mol):
160.4  (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pKₐ:
4.09  (Pearce & Simkins 1968)
3.94  (Schwarzenbach et al. 1988; Haderlein & Schwarzenbach 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: 0.132 (mp at 114.8°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):
6000  (Morrison & Boyd 1959, Howard 1989)
5600  (18°C, Verschureen 1977)
335*  (20 ± 0.5°C, shake flask-UV at pH 1.5, Schwarzenbach et al. 1988)
2787  (20 ± 0.5°C, supercooled liquid S_L, Schwarzenbach et al. 1988)
5000  (selected, Brecken-Folse et al. 1994; Howe et al. 1994)
560  (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
691*  (shake flask-conductimetry, measured range 15.1–35°C, Achard et al. 1996)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.52 × 10⁻³ (Knudsen effusion method, Hoyer & Peperle 1958)
log (P/mmHg) = 13.95 – 5466/(T/K), temp range 20–60°C (Knudsen effusion method, Hoyer & Peperle 1958)
1.987 × 10⁻³ (18°C, Mabey et al. 1982)
5.520 × 10⁻³ (Interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/KPa) = 13.075 – 5466/(T/K), temp range 291–333 K (solid, Antoine eq., Stephenson & Malanowski 1987)
0.111  (20°C: supercooled liquid P_L, GC-RT correlation, Schwarzenbach et al. 1988)
0.0207  (20°C: solid P_S, converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)
log (P_L/atm) = 7.392 – 3680/(T/K) (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

Henry’s Law Constant (Pa·m³/mol at 25°C):
6.54 × 10⁻⁵ (18°C, calculated-P/C, Mabey et al. 1982)
0.00335 (20°C, calculated-P/C, Schwarzenbach et al. 1988)
8.880 × 10⁻⁵ (calculated-P/C, Howard 1989)
Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.53 (Leo et al. 1971)
- 1.50 (shake flask-UV, Stockdale & Selwyn 1971)
- 1.54 (shake flask-GC, Kurihara et al. 1973)
- 1.56 (shake flask-UV, Korenman et al. 1977)
- 1.52 (QSAR, Scherrer & Howard 1979)
- 1.55 (shake flask-UV, Terada et al. 1981)
- 1.79 ± 0.06 (HPLC-RV correlation-ALPM, Garst 1984)
- 1.51 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.67 (21 ± 1.5°C, shake flask-UV, both phases, Schwarzenbach et al. 1988)
- 1.54 (recommended, Sangster 1993)
- 1.53 (22°C, shake flask, Brecken-Folse et al. 1994)
- −0.23 (shake flask, pH 7.5, Howe et al. 1994)
- 1.67 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 1.19 (microorganism-water, calculated, $K_{OW}$, Mabey et al. 1982)
- < 1.0 (calculated, Howard 1989)

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

- 1.22 (sediment-water, calculated, $K_{OW}$, Mabey et al. 1982)
- 1.56, 2.14 (calculated-S, $K_{OW}$, Howard 1989)
- −0.09 (calculated-$K_{OW}$, Kollig 1993)
- 3.09 (activated carbon, Blum et al. 1994)

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

**Volatileization:**

**Photolysis:**

Oxidation: aqueous oxidation rate constants $k = 3 \times 10^4 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, and $k = 5 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxo radical (Mabey et al. 1982);

- $t_\frac{1}{2}$ = 77–3840 h in water, based on reported reaction rate constants for RO$_2$ with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
- $t_\frac{1}{2}$ = 111–1114 h in air, based on the estimated reaction rate constant $k = 1.7 \times 10^{-11} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ with an ambient hydroxyl radical concentration of $8 \times 10^5$ molecules·cm$^{-3}$ for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);
- aqueous photooxidation $t_\frac{1}{2}$ = 200 min in the presence of hydrogen peroxide irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

**Hydrolysis:**

Biodegradation: 95% degradation in 7–10 d in mixed bacteria cultures (Tabak et al. 1964);

- average rate of biodegradation 6.0 mg COD g$^{-1}$$\cdot$h$^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
- first-order rate constant $k = 0.2$ d$^{-1}$ corresponding to a $t_\frac{1}{2} = 3.6$ d in adapted activated sludge under aerobic conditions (Mills et al. 1982);
- aqueous aerobic $t_\frac{1}{2} = 1622–6312$ h, based on data from aerobic soil column studies (Kincannon & Lin 1985; selected, Howard et al. 1991) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);
- aqueous anaerobic $t_\frac{1}{2} = 68–170$ h, based on anaerobic flooded soil die-away tests (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

- $t_\frac{1}{2}$ (aerobic) = 68 d, $t_\frac{1}{2}$ (anaerobic) = 2.8 d in natural waters (Capel & Larson 1995)

**Biotransformation:** bacterial transformation rate constant $k = 3 \times 10^{-9}$ mL·cell$^{-1}$$\cdot$h$^{-1}$ in water (Mabey et al. 1982).

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

**Half-Lives in the Environment:**

Air: calculated vapor-phase $t_\frac{1}{2}$ = 14 h for reaction with photochemically generated OH radical (Howard 1989)
photooxidation $t_{1/2} = 111–1114$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);
atmospheric transformation lifetime was estimated to be $> 5$ d (Kelly et al. 1994).
Surface water: calculated $t_{1/2} = 58$ d for reaction with alkylperoxy radical in water (Howard 1989);
t$_{1/2} = 77–3840$ h, based on reported reaction rate constants for RO$_2$ radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
photooxidation $t_{1/2} = 200$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)
t$_{1/2}$(aerobic) = 69 d, $t_{1/2}$(anaerobic) = 2.8 d in natural waters (Capel & Larson 1995)
Groundwater: $t_{1/2} = 68–14624$ h, based on estimated aqueous aerobic biodegradation half-life and estimated aqueous anaerobic biodegradation half-life (quoted, Howard et al. 1991).
Sediment:
Soil: $t_{1/2} = 1622–6312$ h, based on data from aerobic soil column studies (Kincannon & Lin 1985) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);
a Class C compounds with a $t_{1/2} > 50$ d in soil (Ryan et al. 1988).
t$_{1/2} = 145$ d in sandy loam (Kjeldsen et al. 1990)
Biota:

| TABLE 14.1.3.4.1 |
| Reported aqueous solubilities of 2,4-dinitrophenol at various temperatures |
| Schwarzenbach et al. 1988 | Achard et al. 1996 |
| | shake flask-UV spec. | shake flask-conductimetry |
| $t/\text{°C}$ | $S/\text{g} \cdot \text{m}^{-3}$ | $t/\text{°C}$ | $S/\text{g} \cdot \text{m}^{-3}$ |
| solid | supercooled liquid |
| 5 | 171.8 | 0 | 2019 |
| 10 | 206.6 | 10 | 2213 |
| 20 | 335.0 | 20 | 2852 |
| 30 | 473.2 | 30 | 3199 |

2,4-Dinitrophenol: solubility vs. $1/T$

**FIGURE 14.1.3.4.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4-dinitrophenol.
14.1.3.5 2,4,6-Trinitrophenol (Picric acid)

Common Name: 2,4,6-Trinitrophenol
Synonym: Picric acid
Chemical Name: 2,4,6-trinitrophenol
CAS Registry No: 88-89-1
Molecular Formula: C$_6$H$_3$N$_3$O$_7$, C$_6$H$_2$(NO$_2$)$_3$OH
Molecular Weight: 229.104
Melting Point (°C):
  122.5  (Lide 2003)
Boiling Point (°C):
  > 300  (explodes, Weast 1982–83; Dean 1985; Lide 2003)
Density (g/cm$^3$ at 20°C):
  1.763  (Weast 1982–83; Dean 1985)
Acid Dissociation Constant, pK$_a$:
  0.78  (Schwarzenbach et al. 1988)
Molar Volume (cm$^3$/mol):
  188.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta$H$_{fus}$ (kJ/mol):
  19.50  (Tsonopoulos & Prausnitz 1971)
Entergy of Fusion, $\Delta$S$_{fus}$ (J/mol K):
  49.37  (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming $\Delta$S$_{fus}$ = 56 J/mol K), F:
  0.111  (mp at 122.5°C)
Water Solubility (g/m$^3$ or mg/L at 25°C):
  14000  (Morrison & Boyd 1959)
  13750  (selected, Tsonopoulos & Prausnitz 1971)
  14000  (20°C, Verschueren 1983)
  13000  (Dean 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  $4.68 \times 10^{-5}$ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_v/kPa) = 11.319 – 5560/(T/K)$, temp range 468–598 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
  $7.66 \times 10^{-7}$ (calculated-P/C, this work)
Octanol/Water Partition Coefficient, log K$_{ow}$:
  1.44  (shake flask-GC, Korenman et al. 1977)
  1.34  (Scherrer & Howard 1979)
  1.46  (HPLC-RV correlation, Garst 1984)
  -0.97, 0.87  (shake flask, Log P database: pH 2.7, pH 1, Hansch & Leo 1987)
  2.03  (shake flask, Log P Database, Hansch Leo 1987)
  1.33  (recommended, Sangster 1993)
  1.82  (COMPUTOX databank, Kaiser 1993)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

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

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

- Volatilization:
- Photolysis:
  - Oxidation: photooxidation $t_{1/2} = 677–4320$ h, based on estimated reaction rates with OH and NO$_3$ radicals in air (Howard et al. 1991).
- Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);
  - aqueous aerobic $t_{1/2} = 672–8640$ h, based on aerobic biodegradation screening test (Howard et al. 1991);
  - aqueous anaerobic $t_{1/2} = 48–300$ h, based on aqueous anaerobic natural water die-away test data (Howard et al. 1991)
- Biotransformation:

Half-Lives in the Environmental Compartments:

- Air: $t_{1/2} = 672–4320$ h, based on estimated photooxidation half-lives in air (Howard et al. 1991).
- Surface water: $t_{1/2} = 672–4320$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
- Ground water: $t_{1/2} = 48–8640$ h, based on estimated both aqueous aerobic and aqueous anaerobic biodegradation half-lives (Howard et al. 1991).
- Sediment:
  - Soil: $t_{1/2} = 672–4320$ h, based on estimated photooxidation aqueous aerobic biodegradation half-lives (Howard et al. 1991).
- Biota:
14.1.3.6 4,6-Dinitro-o-cresol

Common Name: 4,6-Dinitro-o-cresol
Synonym: 2,4-dinitro-6-methylphenol, DNOC, 2-methyl-4,6-dinitrophenol, 6-methyl-2,4-dinitrophenol
Chemical Name: 4,6-dinitro-o-cresol, 2,4-dinitro-6-methylphenol
CAS Registry No: 534-52-1
Molecular Formula: C₇H₆N₂O₅, CH₃C₆H₂(NO₂)₂OH
Molecular Weight: 198.133
Melting Point (°C):
86.5 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
312 (Howard 1991)
Density (g/cm³ at 20°C):
Acid Dissociation Constant, pKa:
4.35 (Pearce & Simkins 1968; Callahan et al. 1979; Westall et al. 1985)
4.31 (Schwarzenbach et al. 1988; Howard 1991)
4.46 (Jafvert 1990; quoted, Bintein & Devillers 1994)
Molar Volume (cm³/mol):
182.6 (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: 0.249 (mp at 86.5°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
258, 250 (Günther et al. 1968)
290 (calculated-K_ow, Mabey et al. 1982)
198 (20°C, neutral species at pH 1.5 of buffer solution HCl/NaH₂PO₄, shake flask-UV, Schwarzenbach et al. 1988)
150 (20°C, quoted, Howard 1991)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.048 (35°C, Knudsen effusion method, Hamaker & Kerlinger 1969)
6.670 (20°C, estimated, Mabey et al. 1982)
0.0142 (interpolated-Antoine eq., solid, Stephenson & Malanowski 1987)
log (P_s/kPa) = 13.265 – 5400/(T/K); temp range 290–324 K (Antoine eq., solid, Stephenson & Malanowski 1987)
0.240 (20°C, GC-RT correlation, supercooled liquid value P_L, Schwarzenbach et al. 1988)
0.0432 (20°C, solid P_s, Schwarzenbach et al. 1988)
0.0111 (20°C, quoted, Howard 1991)
Henry’s Law Constant (Pa·m³/mol):
4.050 (calculated-P/C, Mabey et al. 1982)
43.22 (20°C, calculated-P/C, Schwarzenbach et al. 1988)
Octanol/Water Partition Coefficient, log K_ow at 25°C or as indicated:
2.70 (calculated-fragment const., Mabey et al. 1982)
2.12 (21.5°C, neutral species, shake flask-UV, Schwarzenbach et al. 1988)
–0.81 (21.5°C, ionic species at pH 12, Schwarzenbach et al. 1988)
2.12 (Howard 1991)
Phenolic Compounds

2.12 (Sangster 1993)
2.56, 1.98 (COMPUTOX databank, Kaiser 1993)

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

- 2.10 (microorganism-water, calculated-\( K_{OW} \), Mabey et al. 1982)
- 1.38, 1.57 (calculated-S, \( K_{OW} \) regression equations., Howard 1991)

Bioconcentration Factor, log BCF:

- 2.38 (sediment-water, calculated-\( K_{OW} \), Mabey et al. 1982)
- 3.57 ± 0.130 (natural sediment, Jafvert 1990)
- 2.44, 2.0–2.53 (calculated-S, \( K_{OW} \) regression eq., Howard 1991)
- 2.41, 2.78 (soil, quoted, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)
- 3.28 (activated carbon, Blum et al. 1994)

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

- 2.38 (sediment-water, calculated-\( K_{OW} \), Mabey et al. 1982)
- 3.57 ± 0.130 (natural sediment, Jafvert 1990)
- 2.44, 2.0–2.53 (calculated-S, \( K_{OW} \) regression eq., Howard 1991)
- 2.41, 2.78 (soil, quoted, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)
- 3.28 (activated carbon, Blum et al. 1994)

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

Volatile:
- nonvolatile from water, based on low Henry’s law constant value (Howard 1991).

Photolysis:
- Oxidation: aqueous oxidation rate constant \( k = 3 \times 10^4 \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and \( k = 5 \times 10^5 \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical at 25°C (Mabey et al. 1982);
- photooxidation \( t_{1/2} = 77–3840 \text{ h} \) in water, based on reported reaction rate constants for \( \text{RO}_2 \) radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
- photooxidation \( t_{1/2} = 310–3098 \text{ h} \) in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:
- Biodegradation: aqueous aerobic \( t_{1/2} = 168–504 \text{ h} \), based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991); aqueous anaerobic \( t_{1/2} = 68–170 \text{ h} \), based on flooded soil die-away tests for 2,4-dinitrophenol (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)
- \( t_{1/2}^{(\text{aerobic})} = 7 \text{ d}, t_{1/2}^{(\text{anaerobic})} = 28 \text{ d} \) in natural waters (Capel & Larson 1995)

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

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

Half-Lives in the Environment:
- Air: photooxidation \( t_{1/2} = 310–3098 \text{ h} \) in air, based on estimated rate constant for the vapor phase reaction with \( \text{OH} \) radical in air (Atkinson 1987; selected, Howard et al. 1991);
- \( t_{1/2} = 77 \text{ d} \) for the vapor-phase reaction with \( \text{OH} \) radical (conc. of \( 5 \times 10^5 \text{ molecule·cm}^{-3} \)) (Howard 1991); atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).
- Surface water: photooxidation \( t_{1/2} = 77–3840 \text{ h} \) in water, based on reported reaction rate constants for \( \text{RO}_2 \) radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
- \( t_{1/2} = 58 \text{ d} \) estimated for photooxidation via peroxy radicals and \( t_{1/2} = 2600 \text{ yr} \) for reaction with singlet oxygen in water (Howard 1991)
- \( t_{1/2}^{(\text{aerobic})} = 7 \text{ d}, t_{1/2}^{(\text{anaerobic})} = 2.8 \text{ d} \) in natural waters (Capel & Larson 1995)
- Ground water: \( t_{1/2} = 68–1008 \text{ h} \), based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:
- \( t_{1/2} = 168–504 \text{ h} \), based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991).

Biota:
14.1.4 DIHYDROXYBENZENES, METHOXYPHENOLS AND CHLOROGUAIACOLS

14.1.4.1 Catechol (1,2-Dihydroxybenzene)

![Catechol structure](image)

Common Name: Catechol
Synonym: 1,2-dihydroxybenzene, 1,2-benzenediol, pyrocatechol
Chemical Name: 1,2-dihydroxybenzene
CAS Registry No: 120-80-9
Molecular Formula: C₆H₄(OH)₂
Molecular Weight: 110.111
Melting Point (°C): 104.6 (Lide 2003)
Boiling Point (°C): 245 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³): 1.1493 (22 °C, Weast 1982–83)
Acid Dissociation Constant, pKₐ:
- 9.40 (Fieser & Fieser 1958)
- 9.50 (McLeese et al. 1979)
Molar Volume (cm³/mol): 110.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 22.76 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
- 60.25 (Tsonopoulos & Prausnitz 1971)
- 60.21 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.166 (mp at 104.6°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
- 71166 (30°C, synthetic method, Walker et al. 1931)
- 65000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
- 636190 (quoted, Tsonopoulos & Prausnitz 1971)
- 39630 (calculated-K_{ow}, Yalkowsky & Morozowich 1980)
- 42724, 38610 (calculated-ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)
- 43000 (Dean 1985)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 666.6* (104°C, summary of literature data, temp range 104–245.5°C, Stull 1947)
- 1333* (118.5°C, ebulliometry, measured range 118.5–245.5°C, Vonerres et al. 1955)
  \[ \log (P/\text{mmHg}) = -0.2185 \times 13779.7/(T/K) + 8.694319; \text{temp range 104–245.5°C} \] (Antoine eq., Weast 1972–73)
- 1.34 (extrapolated-Antoine eq., Boublik et al. 1973)
  \[ \log (P/\text{mmHg}) = 7.57299 - 2024.422/(186.533 + t/°C); \text{temp range 118.5–245.5°C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1973)
- 5.44 (extrapolated-Antoine eq., Boublik et al. 1984)
  \[ \log (P/\text{mmHg}) = [1 - 517.477/(T/K)] \times 10^4 \{0.902426 - 6.04783 \times 10^{-4} \times (T/K) + 6.58278 \times 10^{-7} \times (T/K)^2 \}; \text{temp range: } 377.15–518.65 \text{ K, (Cox eq., Chao et al. 1983)} \]
- 1.03(extrapolated-Antoine eq., Dean 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C):

0.022 (calculated-P/C)

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

- 0.86 (shake flask-UV, Fujita et al. 1964)
- 0.95 (Leo et al. 1971)
- 0.85 (shake flask-UV, pH 5.6, Umeyama et al. 1971)
- 0.84 (shake flask, Korenman 1972)
- 0.86 (shake flask at pH 7, Unger et al. 1978)
- 0.88, 1.01, 0.85, 0.84 (literature values, Hansch & Leo 1979)
- 0.95 (GC-RT correlation, Veith et al. 1979)
- 1.10 (HPLC-RT correlation, Butte et al. 1981)
- 0.53 (HPLC-RT correlation, Haky & Young 1984)
- 1.10 (HPLC-RT correlation, Webster et al. 1985)
- 0.88 (recommended, LOGKOW databank, Sangster 1993)
- 0.88 (recommended, Hansch et al. 1995)

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

2.03 (soil, calculated-MCI $\chi$, Sabljic et al. 1995)
1.42; 1.74, 2.25, 2.01, 1.98, 1.82 (soil: calculated-$K_{ow}$; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization:

Photolysis:

Oxidation: $t_\frac{1}{2} < 2 \times 10^2$ M⁻¹ s⁻¹ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_\frac{1}{2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_\frac{1}{2} = 2.6–26$ h in air, based on vapor-phase reaction rate constant with OH radical in atmosphere (Howard et al. 1991);

aqueous photooxidation $t_\frac{1}{2} = 77–3840$ h, based on reaction rate constant for RO₂⁻ radical in aqueous solution (Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $k = 55.5$ mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

2 mM catechol rapidly degraded by strain Cat in batch culture in 9 d (Schnell et al. 1989);

aqueous aerobic $t_\frac{1}{2} = 24–168$ h, based on aerobic biological screening test data (Heukelekian & Rand 1955; Okey & Bogan 1965; Pitter 1976; Urushigawa et al. 1983; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_\frac{1}{2} = 96–672$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environmental Compartments:

Air: $t_\frac{1}{2} = 24–168$ h, based on estimated photooxidation half-lives in air (Atkinson 1987; selected, 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 aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Ground water: $t_{1/2} = 48–336$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

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

Biota:

TABLE 14.1.4.1.1
Reported vapor pressures of catechol (1,2-dihydroxybenzene) at various temperatures

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<thead>
<tr>
<th>Summary of literature data</th>
<th>Ebulliometry</th>
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<tr>
<td>Stull 1947</td>
<td>Vonterres et al. 1955</td>
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<tr>
<td>$t/^\circ C$</td>
<td>$P/Pa$</td>
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<td>104.0</td>
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<td>mp/$^\circ C$</td>
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<td>bp/$^\circ C$</td>
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</table>

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**FIGURE 14.1.4.1.1** Logarithm of vapor pressure versus reciprocal temperature for catechol.
14.1.4.2  3,5-Dichlorocatechol

Common Name: 3,5-Dichlorocatechol
Synonym:
Chemical Name: 3,5-dichlorocatechol
CAS Registry No: 13673-92-2
Molecular Formula: C₆H₄Cl₂O₂, C₆H₂Cl₂(OH)₂
Molecular Weight: 179.001
Melting Point (°C):
    83–84  (Varhaníčková 1995)
Boiling Point (°C):
Density (g/cm³):
    7.78  (Varhaníčková 1995)
Molar Volume (cm³/mol):
    152.6  (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₛₐₕ (kJ/mol):
Enthalpy of Fusion, ΔHₕᵤₛ (kJ/mol):
Entropy of Fusion, ΔSₕᵤₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₕᵤₛ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
    7910  (at pH 4.70, shake flask-HPLC/UV, Varhaníčková 1995)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒₖₕ:
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₒₛ:
Environmental Fate Rate Constants, k, and Half-Lives, tₒₖ:
Half-Lives in the Environment:
14.1.4.3 4,5-Dichlorocatechol

Common Name: 4,5-Dichlorocatechol
Synonym: 
Chemical Name: 4,5-dichlorocatechol
CAS Registry No: 3428-24-8
Molecular Formula: C₆H₄Cl₂O₂, C₆H₂Cl₂(OH)₂
Molecular Weight: 179.001
Melting Point (°C):
116–117 (Varhaníčková 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
8.17 (Varhaníčková 1995)
Molar Volume (cm³/mol):
152.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
Enthalpy of Sublimation, ΔHsubl (kJ/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
12000 (at pH 3.20, shake flask-HPLC/UV, Varhaníčková 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations
0.408 (supercooled liquid P_L, GC-RT correlation, Lei et al. 1999)
log (P_L/Pa) = −3680/(T/K) − 11.95, (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.00078 (calculated-P_L/C_L, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kow:
2.51–2.93 (NCASI 1992)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF or log Kᵦ:
1.18–1.51 (estimated-KOW, NCASI 1992)
Sorption Partition Coefficient, log KOC:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
# 3,4,5-Trichlorocatechol

![Chemical Structure](image)

**Common Name:** 3,4,5-Trichlorocatechol  
**Synonym:** 3,4,5-trichloro-1,2-benzenediol  
**Chemical Name:** 3,4,5-trichlorocatechol  
**CAS Registry No:** 56961-20-7  
**Molecular Formula:** C₆H₃Cl₃O₂, C₆HCl₂(OH)₂  
**Molecular Weight:** 213.446  
**Melting Point (°C):**  
- 130 (Varhaníčková 1995)  
- 134 (Lide 2003)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
- 1.735 (Le Bas method-calculated at normal boiling point)  
**Acid Dissociation Constant, pKₐ:** 6.95 (Varhaníčková 1995)  
**Molar Volume (cm³/mol):**  
- 79.3 (Lei et al. 1999)  
**Enthalpy of Vaporization, ΔHᵥ (kJ/mol):**  
- 79.3 (Lei et al. 1999)  
**Enthalpy of Sublimation, ΔHₘₖ (kJ/mol):**  
**Enthalpy of Fusion, ΔHₙ (kJ/mol):**  
**Entropy of Fusion, ΔSₙ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔSₙ = 56 J/mol K), F:** 0.085 (mp at 134°C)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
- 511 (at pH 4.05, shake flask-HPLC/UV, Varhaníčková 1995)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
- 0.106 (supercooled liquid Pt, GC-RT correlation, Lei et al. 1999)  
- log (Pt/Pa) = –4135/(T/K) – 12.89, (GC-RT correlation, Lei et al. 1999)  
**Henry’s Law Constant (Pa m³/mol at 25°C):**  
**Octanol/Water Partition Coefficient, log Kₐₕ:**  
- 3.79, 3.71 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)  
- 3.89, 3.17 (calculated-π constant, fragment constant, Xie et al. 1984)  
- 3.71 (HPLC-RT correlation, Xie et al. 1984; quoted, Sangster 1993)  
- 3.75 (quoted, NCASI 1992)  
**Octanol/Air Partition Coefficient, log Kₐₕ:**  
**Bioconcentration Factor, log BCF or log Kₕ:**  
- 2.16 (estimated-Kₐₕ, NCASI 1992)  
**Sorption Partition Coefficient, log Kₐₕ:**  
- 4.35 (sediment, Kₚ = 22 ml/(kg of organic C)⁻¹, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)  
**Environmental Fate Rate Constants, k, and Half-Lives, tₚ:**  
**Half-Lives in the Environment:**
14.1.4.5 Tetrachlorocatechol

Common Name: Tetrachlorocatechol
Synonym: 3,4,5,6-tetrachloro-1,2-benzenediol
Chemical Name: tetrachlorocatechol
CAS Registry No: 1198-55-6
Molecular Formula: C₆H₂Cl₄O₂, C₆Cl₄(OH)₂
Molecular Weight: 247.891
Melting Point (°C):
194 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
5.83 (Varhaníčková 1995)
Molar Volume (cm³/mol):
194.4 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
77.9 (Lei et al. 1999)
Enthalpy of Sublimation, ΔHₛᵤₜ (kJ/mol):
Enthalpy of Fusion, ΔHₙₑᵤₜ (kJ/mol):
Entropy of Fusion, ΔSₑᵤₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₑᵤₜ = 56 J/mol K), F: 0.022 (mp at 194°C)
Water Solubility (g/m³ or mg/L at 25°C):
70.5 (at pH 5.13, shake flask-HPLC/UV, Varhaníčková 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.068 (supercooled liquid Pᵥ, GC-RT correlation, Lei et al. 1999)
\[ \log (Pᵥ/Pa) = -4070/(T/K) - 12.48, \] (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.035 (calculated-Pᵥ/Cᵥ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kᵥₒₜ₈:
4.29 (shake flask-GC, Fujita et al. 1964)
4.27 (HPLC-RT correlation, Saarikoski & Viluksela 1982)
4.19, 4.27 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)
4.29 (recommended, Sangster 1993)
4.29 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kᵦᵦ:
2.54 (estimated-Kᵥₒₜ₈, NCASI 1992)
Sorption Partition Coefficient, log $K_{OC}$:

4.56  (sediment, $K_p = 36.1 \text{ ml/(kg of organic C0}^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

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

Half-Lives in the Environment:
14.1.4.6 Resorcinol (1,3-Dihydroxybenzene)

Common Name: Resorcinol
Synonym: 1,3-benzenediol, m-dihydroxybenzene, m-hydroxyphenol, resorcin
Chemical Name: 1,3-dihydroxybenzene
CAS Registry No: 108-46-3
Molecular Formula: C₆H₆O₂, C₆H₄(OH)₂
Molecular Weight: 110.111
Melting Point (°C): 109.4 (Lide 2003)
Boiling Point (°C): 276.5 (Lide 2003)
Density (g/cm³): 1.2717 (Weast 1982–83)
Acid Dissociation Constant, pKₐ: 9.40 (Fieser & Fieser 1958; McLeese et al. 1979)
Molar Volume (cm³/mol): 110.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH₉₁₋₂₀ (kJ/mol): 21.30 (Tsonopoulos & Prausnitz 1971)
Entergy of Fusion, ΔS₉₁₋₂₀ (J/mol K): 55.65 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS₉₁₋₂₀ = 56 J/mol K), F: 0.149 (mp at 109.4°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
2188900 (33.6°C, synthetic method, Walker et al. 1931)
1230000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
1390000 (Tsonopoulos & Prausnitz 1971)
840000, 2290000 (0, 30°C, Verschueren 1983)
110000 (Dean 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.3300* (extrapolated-regression of tabulated data, temp range 108.4–276.5°C, Stull 1947)
1333* (151.5°C, ebulliometry, measured range 151.5–276.5°C, Vonteres et al. 1955)
0.0118 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)
log (P/mmHg) = [–0.2185 × 16400.8/(T/K)] + 9.413304; temp range 108.4–276.5°C (Antoine eq., Weast 1972–73)
0.0280* (gas saturation, extrapolated-Antoine eq., measured range 55–106°C, Bender et al. 1983)
log (P/mmHg) = [1– 549.041/(T/K)] × 10^8{0.958295 – 5.78954 × 10^-4·(T/K) + 6.46841 × 10^-7·(T/K)^2}; temp range 381.55–549.65 K (Cox eq., Chao et al. 1983)
0.0515 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.16673 – 2359.273/(180.962 + t/°C); temp range 151.5–216.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
0.0300 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.889 – 2231/(169.0 + t/°C), temp range 151–276°C (Antoine eq., Dean 1985, 1992)
0.0118 (Pₛ, interpolated-Antoine eq.-I, temp range 10–50°C, Stephenson & Malanowski 1987)
log (Pₛ/kPa) = 11.425 – 4876/(T/K); temp range 283–323 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log \( (P_l/kPa) = 6.52635 - 1918.1/(-128.65 + T/K) \); temp range 419–550 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log \( (P_l/kPa) = 6.1041 - 1745.2/(-133.81 + T/K) \); temp range 392–463 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol):
4.0 × 10⁻⁸ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, \( \log K_{ow} \):
- 0.80 (shake flask-UV, Fujita et al. 1964; Leo et al. 1969)
- 0.78 (20°C, shake flask-UV, Korenman 1972)
- 0.80, 0.77, 0.78 (Hansch & Leo 1979)
- 0.77 (shake flask-UV, Beezer et al. 1980)
- 0.88 (shake flask-HPLC both phases, Nahum & Horvath 1980)
- 0.36 (HPLC-RT correlation, Butte et al. 1981)
- 0.77 (shake flask, Log P Database, Hansch & Leo 1987)
- 0.82 (HPLC-RT correlation, Minnick et al. 1988)
- 0.79 (shake flask-UV, pH 2-8, Wang et al. 1989)
- 0.80 (COMPUTOX, Kaiser 1993)
- 0.80 (recommended, Sangster 1993)
- 0.72 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
- 0.80 (recommended, Hansch et al. 1995)

Bioconcentration Factor, \( \log BCF \):

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

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

Volatilization:
- Photolysis: measured pseudo-first-order reaction rate constant \( k = 0.014 \) min⁻¹ for direct photolysis in aqueous solutions with \( t_\frac{1}{2} = 50.7 \) min. (Peijnenburg et al. 1992).
- Photooxidation: rate constant \( k > 3 \times 10^5 \) M⁻¹·s⁻¹ for the reaction with ozone in water using 1 mM \( t \)-BuOH as scavenger at pH 2.0 and 20–23°C in water (Hoigné & Bader 1983a,b).

Hydrolysis:
- Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964); average rate of biodegradation \( k = 57.5 \) mg COD g⁻¹·h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); 2 mM resorcinol solution degraded by strain Re10 within 4 d (Schnell et al. 1989).

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

Half-Lives in the Environmental Compartments:

Air:
- Surface water: \( t_\frac{1}{2} = (50.7 \pm 1.0) \) min for directly photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment:

Soil:

Biota:
TABLE 14.1.4.6.1
Reported vapor pressures of resorcinol (1,3-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947  
Vonterres et al. 1955  
Bender et al. 1983

<table>
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<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
<th>Temperature (°C)</th>
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<td>276.5</td>
<td>101325</td>
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<td>248.0</td>
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<td>mp/°C</td>
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b.p. = 276.5 °C  
m.p. = 109.4 °C

FIGURE 14.1.4.6.1 Logarithm of vapor pressure versus reciprocal temperature for resorcinol.
14.1.4.7 Hydroquinone (1,4-Dihydroxybenzene)

Common Name: Hydroquinone
Synonym: 1,4-benzenediol, \( p \)-dihydroxybenzene, \( p \)-hydroxyphenol, quinol, hydroquinol
Chemical Name: 1,4-dihydroxybenzene
CAS Registry No: 123-31-9
Molecular Formula: \( \text{C}_6\text{H}_4(\text{OH})_2 \)
Molecular Weight: 110.111

Melting Point (°C):
172.4 (Lide 2003)

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

Density (g/cm\(^3\)):
1.328 (15°C, Weast 1982–83)

Acid Dissociation Constant, \( pK_a \):
9.90 (McLeese et al. 1979)

Molar Volume (cm\(^3\)/mol):
110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
27.11 (Tsonopoulos & Prausnitz 1971)

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

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), \( F \): 0.036 (mp at 172.4°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C):
73700 (synthetic method, Walker et al. 1931)
80140 (shake flask-interferometry, Korman & La Mer 1936)
80000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
80750 (selected, Tsonopoulos & Prausnitz 1971)
70000 (Rott et al. 1982; Verschueren 1983; Dean 1985)
86450 (Windholz 1983)

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* (132.4°C, summary of literature data, temp range 132.4–286.2°C, Stull 1947)

\[
\log (P/\text{mmHg}) = \left[ -0.2185 \times 18734.0/(T/K) \right] + 10.309301; \text{ temp range 132.4–286.2°C} \quad \text{(Antoine eq., Weast 1972–73)}
\]

0.00276* (gas saturation, extrapolated - Antoine eq., measured range 68–126°C, Bender et al. 1983)

\[
\log (P/\text{mmHg}) = \left[ 1 - 558.031/(T/K) \right] \times 10^4 \times \left[ 0.941185 - 5.32724 \times 10^{-4}(T/K) + 5.41185 \times 10^{-7} (T/K)^2 \right]; \text{ temp range: 432.25–559.15 K} \quad \text{(Cox eq., Chao et al. 1983)}
\]

0.03940 (extrapolated - liquid, Antoine eq., Boublik et al. 1984)

\[
\log (P/\text{kPa}) = 7.41617 - 2397.626/(194.743 + T/°C); \text{ temp range 159.1–286°C} \quad \text{(Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

0.00255 (\( P_s \), interpolated, Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P_s/\text{kPa}) = 12.585 - 5420/(T/K); \text{ temp range 298–346 K} \quad \text{(Antoine eq.-I, solid, Stephenson & Malanowski 1987)}
\]

\[
\log (P_s/\text{kPa}) = 7.00575 - 2321.92/(-95.235 + T/°C); \text{ temp range 448–559 K} \quad \text{(Antoine eq.-II, liquid, Stephenson & Malanowski 1987)}
\]
Henry’s Law Constant (Pa·m³/mol at 25°C):  
3.89 × 10⁻⁶ (quoted, Meylan & Howard 1991)  
5.91 × 10⁻⁶ (estimated-bond contribution, Meylan & Howard 1991)  
4.00 × 10⁻⁶ (calculated-P/C, this work)  

Octanol/Water Partition Coefficient, log $K_{ow}$:  
0.59  
(Leo et al. 1971)  
0.495  
(shake flask-UV at pH 5.62, Umeyama et al. 1971)  
0.59  
(shake flask-GC, Kurihara et al. 1973)  
0.61  
(20°C, shake flask, Korenman 1974)  
0.55, 0.59  
0.61  
(HPLC-RT correlation, Nahum & Horvath 1980)  
0.54  
(shake flask-HPLC, Nahum & Horvath 1980)  
0.99  
(HPLC-RT correlation, Fujisawa & Masuhara 1981)  
0.50  
(shake flask, Log P Database, Hansch & Leo 1987)  
0.50  
(centrifugal partition chromatography CPC, Berthod et al. 1988)  
0.59  
(shake flask, Wang et al. 1989)  
0.59  
(recommended, Sangster 1993)  
0.59  
(recommended, Hansch et al. 1995)  

Bioconcentration Factor, log $BCF$:  
1.81  
(green algae, *Chlorella*, exposure to 50 µg/L for 24 h, Geyer et al. 1981)  
0.95  
(calculated-S, Geyer et al. 1981)  
1.60, 2.72  
(golden orfe, activated sludge, Freitag et al. 1982)  
1.60, 1.60  
(algae, fish, Freitag et al. 1984)  
1.54  
(algae, wet weight basis after 1 d, Geyer et al. 1984)  
0.602  
(calculated-$K_{ow}$, Geyer et al. 1984)  
2.93  
(activated sludge, Freitag et al. 1987)  

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

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:  

Volatilization:  

Photolysis:  

Oxidation: $k = 1 \times 10^6$ M⁻¹ s⁻¹ for the reaction with RO₂ radical at 30°C in aquatic systems with $t_\text{½} = 12$ min (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);  
$k < 2 \times 10^3$ M⁻¹ s⁻¹ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_\text{½} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);  
aqueous photooxidation $t_\text{½} = 0.39–19.3$ h in surface water, based on measured rate data for the reaction with alkyl peroxy radical in aqueous solution (Mill 1982; selected, Howard et al. 1991);  
photooxidation $t_\text{½} = 6–26.1$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991);  
72.1 mg/L of total organic carbon (TOC) degraded to 98% TOC after 5 h of illumination with a 250 W tungsten lamp by photo-Fenton reaction (Ruppert et al. 1993).  

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

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);  
average rate of biodegradation 54.2 mg COD g⁻¹·h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);  
aqueous aerobic $t_\text{½} = 24–168$ h, based on aqueous screening test data (Ludzack & Ettinger 1960; Belly & Goodhue 1976; Gerike & Fischer 1979; selected, Howard et al. 1991);  
aqueous anaerobic $t_\text{½} = 96–672$ 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 Environmental Compartments:

Air: photooxidation $t_{1/2} = 6–26.1$ 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 to 5 d (Kelly et al. 1994).

Surface water: aqueous photooxidation $t_{1/2} = 0.39–19.3$ h, based on measured rate data for the reaction with alkylperoxyl radical in aqueous solution (Mill 1982; quoted, 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 unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

<table>
<thead>
<tr>
<th>TABLE 14.1.4.7.1</th>
<th>Reported vapor pressures of hydroquinone (1,4-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations</th>
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<tbody>
<tr>
<td>log $P = A - B/(T/K)$</td>
<td>$\ln P = A - B/(T/K)$</td>
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<td>log $(P/mmHg) = A - B/(C + t/°C)$</td>
<td>$\ln P = A - B/(C + t/°C)$</td>
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<tr>
<td>log $(P/Pa) = A - B/(C + T/K)$</td>
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</table>

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FIGURE 14.1.4.7.1 Logarithm of vapor pressure versus reciprocal temperature for hydroquinone.
14.1.4.8 2-Methoxyphenol (Guaiacol)

![Structure of 2-Methoxyphenol](image)

Common Name: Guaiacol  
Synonym: 2-methoxyphenol, methylcatechol, o-hydroxyanisole, 1-hydroxy-2-methoxybenzene, pyrocatechol monomethylether  
Chemical Name: o-methoxyphenol  
CAS Registry No: 90-05-1  
Molecular Formula: C₇H₈O₂, C₆H₄(OCH₃)OH  
Molecular Weight: 124.138  
Melting Point (°C):  
32 (Stephenson & Malanowski 1987; Lide 2003)  
Boiling Point (°C): 204–206  
205 (Lide 2003)  
Density (g/cm³):  
1.129 (crystal)  
1.112 (liquid, solidified at 28°C)  
Acid Dissociation Constant, pK:  
Molar Volume (cm³/mol):  
134.7 (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 = 5 J/mol K), F: 0.854 (mp at 32°C)  
Water Solubility (g/m³ or mg/L at 25°C or as indicated):  
143000–16700 (Windholz 1983)  
16000 (15°C, Verschueren 1983)  
15000 (room temp., Dean 1985)  
18700, 1316 (15°C, 37°C, Yalkowsky et al. 1987)  
24800 (25°C, shake flask-HPLC/UV, Tam et al. 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):  
133.3* (52.4°C, summary of literature data, temp range 52.4–205°C, Stull 1947)  
1333* (82.0°C, ebulliometry, measured range 82.0–205.0°C, Vonterres et al. 1955)  
log (P/mmHg) = [–0.2185 × 13425.8/(T/K)] + 9.027299; temp range 52.4–205°C (Antoine eq., Weast 1972–73)  
log (P/mmHg) = [1– 477.010/(T/K)] × 10^{0.858892 – 4.47192 × 10 –4·(T/K) + 3.228549 × 10–7·(T/K)^2}; temp range 355.15–478.15 K (Cox eq., Chao et al. 1983)  
13.73 (Verschueren 1983)  
8.88 (extrapolated-Antoine eq., Boublik et al. 1984)  
log (P/kPa) = 5.40415 – 1121.391/(125.407 + t°C); temp range 82–205°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
6.79 (extrapolated-Antoine eq., Dean 1985)  
log (P/mmHg) = 6.161 – 1051/(116.0 + t°C); temp range 82–205°C (Antoine eq., Dean 1985, 1992)  
24.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
log (P_kPa) = 6.44572 – 1786.15/(–76.43 + T/K); temp range 378–479 K (Antoine eq., Stephenson & Malanowski 1987)  
21.00 (quoted, Sagebiel & Seiber 1993)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
0.30 (calculated-P/C, Sagebiel et al. 1992)
0.13, 0.11 (gas stripping-UV, headspace-GC, Sagebiel et al. 1992)
0.132 (bubble chamber, Sagebiel & Seiber 1993)
0.049 (calculated-group contribution, Lee et al. 2000)
0.0724 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
\[ \log K_{AW} = 6.198 - \frac{3144}{(T/K)} \] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, \( \log K_{ow} \):
- 1.33 (shake flask-UV, Umeyama et al. 1971)
- 1.35 (shake flask-UV, Korenman 1973)
- 1.33 (shake flask-UV, Norrington et al. 1975)
- 1.58 (Hansch & Leo 1979)
- 1.25 (HPLC-RT correlation, Butte et al. 1981)
- 1.32 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.32 (recommended, LOGKOW databank, Sangster 1993)
- 1.32 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{oc} \):
- 1.56 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 14.1.4.8.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of 2-methoxyphenol (guaiacol) at various temperatures</td>
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FIGURE 14.1.4.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methoxyphenol (guaiacol).
14.1.4.9 3-Methoxyphenol

Common Name: 3-Methoxyphenol
Synonym: m-methoxyphenol, m-hydroxyanisole, resorcinol monomethylether
Chemical Name: 3-methoxyphenol
CAS Registry No: 150-19-6
Molecular Formula: CH₃OC₆H₄OH
Molecular Weight: 124.138
Melting Point (°C): < –17 (Lide 2003)
Boiling Point (°C): 244 (Stephenson & Malanowski 1987)
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
134.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
67800 (shake flask-HPLC/UV, Varhaníčková et al. 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.262 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_r/kPa) = 6.12536 – 1572.51/(–136.16 + T/K); temp range 413–518 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa-m³/mol at 25°C):
0.10 (estimated as per Sagebiel et al. 1992 data on 2-methoxyphenol)
Octanol/Water Partition Coefficient, log K₀W:
1.58 (Leo et al. 1969; Hansch & Leo 1979)
1.47 (HPLC-k correlation, Minick et al. 1988)
1.58 (COMPUTOX databank, Kaiser 1993)
1.58 (recommended, Hansch et al. 1995)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_OC:
1.50 (soil, calculated-MCI ‘χ, Sabljic et al. 1995)
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Half-Lives in the Environment:
14.1.4.10 4-Methoxyphenol

Common Name: 4-Methoxyphenol
Synonym: p-methoxyphenol, p-hydroxyanisole, hydroquinone monomethylether
Chemical Name: 4-methoxyphenol
CAS Registry No: 150-76-5
Molecular Formula: CH₃OC₆H₄OH
Molecular Weight: 124.138

Melting Point (°C):
  57  (Lide 2003)

Boiling Point (°C):
  243  (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³):

Acid Dissociation Constant, pKₐ:

Molar Volume (cm³/mol):
  134.7  (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: 0.485 (mp at 57°C)

Water Solubility (g/m³ or mg/L at 25°C):
  40000  (Verschueren 1977, 1983)
  19500  (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.033  (extrapolated-Antoine eq., Boublik et al. 1984)
  0.556  (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_s/kPa) = 12.27865 – 4631.266/(T/K); temp range 278–300 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P_s/kPa) = 6.8462 – 2111.03/(-81.56 + T/K); temp range 418–518 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

0.979  (supercooled liquid P_s, GC-RT correlation, Lei et al. 1999)
log (P_s/Pa) = –3664/(T/K) + 12.28 (GC-RT correlation, Lei et al. 1999)

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

Octanol/Water Partition Coefficient, log K_{OW}:
  1.34  (shake flask-UV, Fujita et al. 1964)
  1.37  (shake flask-UV at pH 7.45, Umeyama et al. 1971)
  1.34, 1.33, 1.37 (lit. values, Hansch & Leo 1979)
  1.47  (shake flask, Korenman et al. 1980)
  1.62  (HPLC-k′ correlation, Miyake & Terada 1982)
  1.24  (HPLC-k correlation, Minick et al. 1988)
  1.34  (recommended, LOGKOW databank, Sangster 1993)
  1.34  (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
14.1.4.11 4-Chloroguaiacol

Common Name: 4-Chloroguaiacol
Synonym: 4-chloromethoxyphenol
Chemical Name: 4-chloroguaiacol, 4-chloromethoxyphenol
CAS Registry No: 16766-30-6
Molecular Formula: C_7H_7ClO_2
Molecular Weight: 158.582
Melting Point (°C): liquid
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pK_a:
Molar Volume (cm³/mol):
155.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol·K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol·K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
5140 (shake flask-HPLC/UV, pH 2.8, Tam et al. 1994)
5604 (shake flask-GC/ECD, pH 2.8, Tam et al. 1994)
5370 (selected, Tam et al. 1994)
5132; 13200, 10500 (quoted exper.; calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)

Vapor Pressure (Pa at 25°C):

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

Octanol/Water Partition Coefficient, log K_ow:
2.15 (calculated-fragment const., Niimi et al. 1990)
2.11–2.52 (literature range, NCASI 1992)

Bioconcentration Factor, log BCF:
0.0 (trout, 1–21 d exposure, BCF < 1, Niimi et al. 1990)
0.86–1.19 (quoted, NCASI 1992)

Sorption Partition Coefficient, log K_oc:
TABLE 14.1.4.11.1
Reported aqueous solubilities of 4-chloroguaiacol at various temperatures

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FIGURE 14.1.4.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chloroguaiacol.
14.1.4.12 4,5-Dichloroguaiacol

Common Name: 4,5-Dichloroguaiacol
Synonym: 4,5-dichloro-2-methoxyphenol
Chemical Name: 4,5-dichloroguaiacol
CAS Registry No: 2460-49-3
Molecular Formula: C₇H₆Cl₂O₂
Molecular Weight: 193.028
Melting Point (°C): 69–70
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
   8.26, 8.52  (20°C, regressions, Xie & Dyrsen 1984)
Molar Volume (cm³/mol):
   176.5  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H₉₅ (kJ/mol):
Entropy of Fusion, ∆S₉₅ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S₉₅ = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
   584  (shake flask-HPLC/UV, pH 5.6, Tam et al. 1994)
   565  (shake flask-GC/ECD, pH 5.6, Tam et al. 1994)
   3130, 1086  (supercooled liquid values: calculated-group contribution, calculated- AQUAFAC, Lee et al. 2000)

Vapor Pressure (Pa at 25°C):
   1.54  (supercooled liquid P₉₅, correlated-GC-RT, Bidleman & Renberg 1985)

Henry’s Law Constant (Pa·m³/mol at 25°C):
   0.44  (calculated-Pₗ/Cₗ, Lei et al. 1999)

Octanol/Water Partition Coefficient, log Kₐw:
   3.04  (calculated-fragment const., Rekker 1977)
   3.28  (Hansch & Leo 1979)
   3.26  (shake flask-UV, Saarikoski & Viluksela 1982)
   3.18  (shake flask-GC, Xie et al. 1984)
   3.28  (HPLC-k’ correlation, Xie et al. 1984)
   3.20, 3.19, 3.19  (shake flask-GC, regressions, Xie & Dryszen 1984)
   3.26  (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log Kₒₐ:

Bioconcentration Factor, log BCF or log Kₒᵢ:
   1.74–2.05, 2.03  (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
   1.51, 1.75  (quoted, estimated, NCASI 1992)
   2.03  (Oncorhynchus mykiss, quoted, Devillers et al. 1996)

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

- Volatilization:
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biodegradation: 5% reduction in concn \((5 - M)\) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d (Neilson et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:
14.1.4.13 3,4,5-Trichloroguaiacol

Common Name: 3,4,5-Trichloroguaiacol
Synonym: 3,4,5-trichloro-2-methoxyphenol
Chemical Name: 3,4,5-trichloroguaiacol
CAS Registry No: 57057-83-7
Molecular Formula: C₇H₅Cl₃O₂
Molecular Weight: 227.473
Melting Point (°C): 85–86
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, $pK_a$:
  7.55  (Könemann 1981)
  7.43, 7.52, 7.56 (20°C, regressions, Xie & Dyrssen 1984)
  7.90  (Leuenberger et al. 1985)
  7.56  (Xie et al. 1986)
Molar Volume (cm³/mol):
  197.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  305  (shake flask-HPLC/UV, pH 5.9, Tam et al. 1994)
  313  (shake flask-GC/ECD, pH 5.9, Tam et al. 1994)
Vapor Pressure (Pa at 25°C):
  0.64  (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  0.12  (calculated-P/C, Lei et al. 1999)
Octanol/Water Partition Coefficient, log $K_{ow}$:
  3.77  (shake flask-UV, Saarikoski & Viluksela 1982)
  4.11  (shake flask-GC, Xie et al. 1984)
  4.18  (HPLC-$k'$ correlation, Xie et al. 1984)
  4.14  (shake flask-GC, Xie & Dyrssen 1984)
  3.77  (recommended, Sangster 1993)
  3.77  (COMPUTOX databank, Kaiser 1993)
Octanol/Air Partition Coefficient, log $K_{oa}$:
Bioconcentration Factor, log BCF or log $K_b$:
  1.60  (rainbow trout, Oikari et al. 1985)
  2.06–2.51, 2.41 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
  1.78–1.95  (field studies, bile of rainbow trout, Niimi et al. 1990)
  2.47  (estimated, NCASI 1992)
  2.20  (Oncorhynchus mykiss, Devillers et al. 1996)
Sorption coefficient, $\log K_{OC}$:

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

Half-Lives in the Environment:
- Biota: $t_{1/2} = 1–2$ d in bleak and $t_{1/2} = 2$ d in trout (Niimi et al. 1990).
14.1.4.14 4,5,6-Trichloroguaiacol

Common Name: 4,5,6-Trichloroguaiacol
Synonym: 2,3,4-trichloro-6-methoxyphenol
Chemical Name: 4,5,6-trichloroguaiacol
CAS Registry No: 2668-24-8
Molecular Formula: C\textsubscript{7}H\textsubscript{5}Cl\textsubscript{3}O\textsubscript{2}
Molecular Weight: 227.473
Melting Point (°C): 112–115
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Acid Dissociation Constant, pK\textsubscript{a}: 7.07 (Leuenberger et al. 1985) 7.20 (20°C, regressions, Xie & Dyrssen 1984)
Molar Volume (cm\textsuperscript{3}/mol):
197.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), $F$:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
57.0 (shake flask-HPLC/UV, pH 5.8, Tam et al. 1994) 50.0 (shake flask-GC/ECD, pH 5.8, Tam et al. 1994)
Vapor Pressure (Pa at 25°C):
0.249 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
8.82 (calculated-P/C) 0.14 (calculated-P/C, Lei et al. 1999)
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
Octanol/Air Partition Coefficient, log $K_{\text{oa}}$:
Bioconcentration Factor, log $BCF$:
2.60 (bleaks, Renberg et al. 1980) 1.90–2.11 (rainbow trout, Oikari et al. 1985) 2.59 (bleaks, Walden et al. 1986)
1.88–2.05, 1.97 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
1.78–1.95 (field studies, bile of trout, Niimi et al. 1990)
4.81 (fourhorn sculpin *myoxocephalus quadricornis*, bile BCF in brackish water, during 6–20 d exposure under continuous water-flow conditions, Wachtmeister et al. 1991)
2.22 (estimated, NCASI 1992)
1.97 (*Oncorhynchus mykiss*, Devillers et al. 1996)

Sorption Partition Coefficient, log $K_{OC}$:
3.11 (sediment, $K_p = 1.3$ ml·(kg of organic C)$^{-1}$, batch sorption equilibrium, Remberger et al. 1986, quoted, Neilson et al. 1991)
2.80, 2.94 (soil, quoted, calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
2.80 (soil, calculated-MCI $1\chi$, Sabljic et al. 1995)
1.35 (sediment, $K_p = 22$ ml kg of organic C$^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: 16% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)
Biotransformation:
Bioconcentration, Uptake($k_1$) and Elimination ($k_2$) Rate Constants Rates:

Half-Lives in the Environment:
Biota: $t_{1/2} = 1$ to 2 d in bleak (Niimi et al. 1990).
14.1.4.15 3,4,5,6-Tetrachloroguaiacol

Common Name: 3,4,5,6-Tetrachloroguaiacol
Synonym: 2,3,4,5-tetrachloro-6-methoxyphenol
Chemical Name: 3,4,5,6-tetrachloroguaiacol
CAS Registry No: 2539-17-5
Molecular Formula: C\(_7\)H\(_4\)Cl\(_4\)O\(_2\)
Molecular Weight: 261.918
Melting Point (°C): 121–122
Boiling Point (°C):
Density (g/cm\(^3\)):
Acid Dissociation Constant, pK\(_a\):
   6.26  (Leuenberger et al. 1985)
   6.19, 6.12, 6.26 (20°C, regressions, Xie & Dyrssen 1984)
Molar Volume (cm\(^3\)/mol):
   218.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:
Water Solubility (g/m\(^3\) or mg/L at 25°C):
   27.0  (shake flask-HPLC/UV, pH 4.2, Tam et al. 1994)
   25.0  (shake flask-GC/ECD, pH 4.2, Tam et al. 1994)
   165, 28  (supercooled liquid values: calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)
Vapor Pressure (Pa at 25°C):
   0.138  (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
   1.013  (Leuenberger et al. 1985; quoted, Barton 1987)
   0.15  (calculated-P/C, Lei et al. 1999)
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
   4.29  (Saarikoski & Viluksela 1982)
   4.45  (shake flask-GC, Xie et al. 1984)
   4.76, 5.01, 4.52  (HPLC-k’ correlation, calculated-π const., calculated-fragment const., Xie et al. 1984)
   4.41, 4.43, 4.42  (shake flask, regressions, Xie & Dyrssen 1984)
   4.53  (Leuenberger et al. 1985)
   4.28  (calculated-fragment, Niimi et al. 1990)
   4.59  (COMPUTOX databank, Kaiser 1993)
   4.42, 4.76  (literature values, Sangster 1993)
   4.42  (selected, Hansch et al. 1995)
   3.83  (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):
Bioconcentration Factor, log BCF:
   2.60  (bleaks, after 2 weeks exposure, Renberg et al. 1980)
   1.60–2.18  (rainbow trout, Oikari et al. 1985)
1.78–1.95 (bile of rainbow trout, field studies, Niimi et al. 1990)
2.04–2.38, 2.26 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
3.20 (roach, Niimi et al. 1990, quoted, NCASI 1992)
2.84 (estimated, NCASI 1992)
2.26 (Oncorhynchus mykiss, Devillers et al. 1996)

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

- 2.85 (soil, Seip et al. 1986)
- 3.15 (sediment, \( K_P = 1.5 \) ml·(kg of organic C)\(^{-1} \), batch sorption equilibrium, Remberger et al. 1986)
- 2.30 (soil, calculated-MCI \( \chi \), Bahnick & Doucette 1988)
- 2.85, 3.17 (soil, quoted, calculated-MCI \( \chi \) and fragment contribution, Meylan et al. 1992)
- 2.85 (soil, calculated-MCI \( \chi \), Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 100% reduction in concn (5 -M) after incubation with cells of \( Rhodococcus \) chlorophenolicus for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:

Biota: \( t_{1/2} < 10 \) d in trout liver (Niimi et al. 1990); \( t_{1/2} = 1–2 \) d in bleak (Niimi et al. 1990).
14.1.4.16 Vanillin (4-Hydroxy-3-methoxybenzaldehyde)

Chemical Name: 4-hydroxy-3-methoxybenzaldehyde
Synonym: 4-hydroxy-3-methoxybenzaldehyde, vanillyl aldehyde, methylprotocatechuic aldehyde
CAS Registry No: 121-33-5
Molecular Formula: C_8H_8O_3, C_6H_3OHCHO(OCH_3)
Molecular Weight: 152.148

Melting Point (°C):
81.5 (Lide 2003)

Boiling Point (°C):
285 (Weast 1982–83; Lide 2003)
284 (decomposes, Stephenson & Malanowski 1987)

Density (g/cm³):
1.056 (Weast 1982–83)

Acid Dissociation Constant, pK_a:
7.40 (Sangster 1993)
7.62 (Varhaníčková et al 1995)

Molar Volume (cm³/mol):
156.9 (Le Bas method-calculated 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: 0.279 (mp at 81.5°C)

Water Solubility (g/m³ or mg/L at 25°C):
2480 (at pH 4.50, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
133.3 (107°C, summary of literature data, temp range 107–285°C, Stull 1947)

log (P_v/kPa) = 10.997 – 4623/(T/K); temp range 288–333 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_v/kPa) = 10.93562 – 4535.023/(T/K); temp range 297–328 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_v/kPa) = 7.01734 – 3198.18/(-17.047 + T/K); temp range 380–558 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_v/mmHg) = –25.583 – 4.086 × 10³/(T/K) + 17.515·log (T/K) – 2.8177 × 10⁻²·(T/K)²; temp range 355–777 K (vapor pressure eq., Yaws 1994)

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

Octanol/Water Partition Coefficient, log K_{ow}:
1.31 (shake flask-UV, Korenman & Sotnikova 1975)
1.21 (shake flask-UV, Holmes & Lough 1976)
1.21 (shake flask-HPLC, Bazaco & Coca 1989)
1.21 (recommended, Sangster 1993)
1.21 (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, $t_\text{1/2}$:

Half-Lives in the Environment:
14.1.4.17 5-Chlorovanillin

Common Name: 5-Chlorovanillin
Synonym:
Chemical Name: 5-chlorovanillin
CAS Registry No: 19463-48-0
Molecular Formula: C₈H₇ClO₃, C₆H₂ClCHO(OCH₃)
Molecular Weight: 185.593
Melting Point (°C):
165 (Weast 1982–83; Lide 2003)
169 (Varhaníčková et al 1995)
Boiling Point (°C):
Acid Dissociation Constant, pKₐ
6.80 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
177.8 (Le Bas method –calculated at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
Enthalpy of Sublimation, ∆Hₘₘ (kJ/mol):
Enthalpy of Fusion, ∆Hₖₘ (kJ/mol):
Entropy of Fusion, ∆Sₖₘ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₖₘ = 56 J/mol K), F: 0.042 (mp at 165°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):
932 (at pH 4.55, shake flask-HPLC/UV, Varhaníčková et al 1995)
249* (24°C, shake flask-HPLC/UV, measured range 7.5–85.9°C, Larachi et al. 2000)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐw:
1.76 (NCASI 1992)
Octanol/Air Partition Coefficient, log Kₐₐ:
Bioconcentration Factor, log BCF or log K₆:
0.59 (estimated-K₉₆, NCASI 1992)
Sorption Partition Coefficient, log Kₐₙ:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
TABLE 14.1.4.17.1
Reported aqueous solubilities of 5-chlorovanillin at various temperatures

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
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<tbody>
<tr>
<td>7.5</td>
<td>171</td>
</tr>
<tr>
<td>12.0</td>
<td>171</td>
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<tr>
<td>16.8</td>
<td>184</td>
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<tr>
<td>19.8</td>
<td>168</td>
</tr>
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<td>24.0</td>
<td>249</td>
</tr>
<tr>
<td>30.0</td>
<td>286</td>
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<tr>
<td>36.5</td>
<td>505</td>
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<tr>
<td>46.0</td>
<td>629</td>
</tr>
<tr>
<td>50.0</td>
<td>760</td>
</tr>
<tr>
<td>59.0</td>
<td>932</td>
</tr>
<tr>
<td>65.0</td>
<td>1139</td>
</tr>
<tr>
<td>70.0</td>
<td>1267</td>
</tr>
<tr>
<td>80.0</td>
<td>1767</td>
</tr>
<tr>
<td>85.9</td>
<td>2314</td>
</tr>
</tbody>
</table>

$\Delta S_{\text{fus}}/(\text{kJ mol}^{-1}) = 89.1$

FIGURE 14.1.4.17.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 5-chlorovanillin.
14.1.4.18 6-Chlorovanillin

Common Name: 6-Chlorovanillin
Synonym:
Chemical Name: 6-chlorovanillin
CAS Registry No: 18268-76-3
Molecular Formula: C_8H_7ClO_3, C_6H_2ClCHO(OCH_3)
Molecular Weight: 185.593
Melting Point (°C):
171–172 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pK_a:
6.11 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
177.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Sublimation, ΔH_sub (kJ/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
132 (at pH 5.35, shake flask-HPLC/UV, Varhaníčková et al 1995)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_ow:
1.76 (NCASI 1992)
Octanol/Air Partition Coefficient, log K_OA:
Bioconcentration Factor, log BCF or log K_B:
0.59 (estimated-K_ow, NCASI 1992)
Sorption Partition Coefficient, log K_OC:
Environmental Fate Rate Constants, k, and Half-Lives, t_½:
Half-Lives in the Environment:
14.1.4.19 5,6-Dichlorovanillin

Common Name: 5,6-Dichlorovanillin
Synonym:
Chemical Name: 5,6-dichlorovanillin
CAS Registry No: 18268-69-4
Molecular Formula: C₈H₆Cl₂O₃, C₆HCl₂CHO(OCH₃)
Molecular Weight: 221.038
Melting Point (°C):
198–199 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
5.28 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
198.7 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
Enthalpy of Sublimation, ΔHₙₕ (kJ/mol):
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):
23.0 (at pH 4.0, shake flask-HPLC/UV, Varhaníčková et al 1995)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₒₕw:
2.47 (NCASI 1992)
Octanol/Air Partition Coefficient, log Kₒₕa:
Bioconcentration Factor, log BCF or log Kₒᵢ:
1.76 (estimated, Kₒₕw, NCASI 1996)
Sorption Partition Coefficient, log Kₒᵢc:
Environmental Fate Rate Constants, k, and Half-Lives, t₁/₂:
Half-Lives in the Environment:
14.1.4.20 Syringol (2,6-Dimethoxyphenol)

Common Name: Syringol
Synonym: 2,6-dimethoxyphenol
Chemical Name: 2,6-dimethoxyphenol
CAS Registry No: 91-10-1
Molecular Formula: C_{8}H_{10}O_{3}, C_{6}H_{3}OH(OCH_{3})_{2}
Molecular Weight: 154.163
Melting Point (°C):
  - 56.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pK_{a}:
Molar Volume (cm³/mol):
  - 166.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_{v} (kJ/mol):
Enthalpy of Sublimation, ΔH_{sub} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
  - 18200 (shake flask-UV spectroscopy, Sagebiel & Seiber 1993)
Vapor Pressure (Pa at 25°C):
  - 0.45 (GC-RT correlation, Sagebiel & Seiber 1993)
Henry’s Law Constant (Pa m³/mol at 25°C):
  - 0.00271 (gas stripping-GC, Sagebiel & Seiber 1993)
Octanol/Water Partition Coefficient, log K_{ow}:
  - 1.15 (shake flask-UV, Fujita et al. 1964)
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, tₜ:
Half-Lives in the Environment:
14.1.4.21 3-Chlorosyringol

Common Name: 3-Chlorosyringol
Synonym: 3-chloro-2,6-dimethoxyphenol
Chemical Name: 3-chlorosyringol
CAS Registry No: 18113-22-9
Molecular Formula: C₈H₉ClO₃, C₆H₂(OH)Cl(OCH₃)₂
Molecular Weight: 188.608
Melting Point (°C): 35-36 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
9.09 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
186.9 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
68.6 (Lei et al. 1999)
Enthalpy of Sublimation, ΔHₛₜₜ (kJ/mol):
Enthalpy of Fusion, ΔHₜₜ (kJ/mol):
Entropy of Fusion, ΔSₜₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₜₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
5170 (at pH 4.30, shake flask-HPLC/UV, Varhaníčková et al 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.825 (supercooled liquid Pᵥ, GC-RT correlation, Lei et al. 1999)
log (Pᵥ/Pa) = –3580/(T/K) – 11.93 (GC-RT correlation, Lei et al. 2001)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.011 (calculated-Pᵥ/Cᵥ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kᵥw:
Octanol/Air Partition Coefficient, log Kᵥα:
Bioconcentration Factor, log BCF or log K₉:
Sorption Partition Coefficient, log Kᵥw:
Environmental Fate Rate Constants, k, and Half-Lives, t₀:
Half-Lives in the Environment:
14.1.4.22 3,5-Dichlorosyringol

Common Name: 3,5-Dichlorosyringol
Synonym: 3,5-dichloro-2,6-dimethoxyphenol
Chemical Name: 3,5-dichlorosyringol
CAS Registry No: 78782-46-4
Molecular Formula: C8H8Cl2O2, C6H(OH)Cl2(OCH3)2
Molecular Weight: 223.054
Melting Point (°C):
105–106 (Varhaníčková et al. 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constants, pKₐ:
7.27 (Varhaníčková et al. 1995)
Molar Volume (cm³/mol):
207.8 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
70.4 (Lei et al. 1999)
Enthalpy of Sublimation, ΔHₜₚ (kJ/mol):
Enthalpy of Fusion, ΔHₚₛₜ (kJ/mol):
Entropy of Fusion, ΔSₚₛₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₚₛₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
244 (at pH 5.80, shake flask-HPLC/UV, Varhaníčková et al. 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.465 (supercooled liquid Pᵥ, GC-RT correlation, Lei et al. 1999)
log (Pᵥ/Pₐ) = –3679/(T/K) – 12.01, (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.069 (calculated-Pᵥ/Cᵥ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kₒₒₚ:
Octanol/Air Partition Coefficient, log Kₒₒ₈:
Bioconcentration Factor, log BCF or log Kₚ:
Sorption Partition Coefficient, log Kₒₒₐ:
Environmental Fate Rate Constants, k, and Half-Lives, tₛ:
14.1.4.23  Trichlorosyringol

Common Name: Trichlorosyringol
Synonym: 3,4,5-trichloro-2,6-dimethoxyphenol
Chemical Name: 3,4,5-trichloro-2,6-dimethoxyphenol
CAS Registry No: 2539-26-6
Molecular Formula: C₈H₇Cl₃O₃, C₆(OH)Cl₃(OCH₃)₂
Molecular Weight: 257.499
Melting Point (°C):
   122–123 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
   7.73 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
   228.7 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
   77.4 (Lei et al. 1999)
Enthalpy of Sublimation, ΔHₛₘₙ (kJ/mol):
Enthalpy of Fusion, ΔHₖₜₚₜ = 56 J/mol K
Fugacity Ratio at 25°C (assuming ΔSₖₜₚₜ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
   100 (at pH 3.90, shake flask-HPLC/UV, Varhaníčková et al 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   0.077 (supercooled liquid Pᵥ, GC-RT correlation; Lei et al. 1999)
   log (Pᵥ/Pₐ) = –4014/(T/K) – 12.44, (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
   0.022 (calculated-Pᵥ/Cᵥ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kₖ₉ₕ:
   3.74 (shake flask-GC, Saarikoski & Viluksela 1982)
   4.20 (quoted, NCASI 1992)
   3.74 (recommended, Sangster 1993)
   3.74 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₖ₉ₐ:
Bioconcentration Factor, log BCF or log K₉ₚ:
   1.19 (estimated-Kₖ₉ₕ, NCASI 1992)
Sorption Partition Coefficient, log Kₖ₉ₜ:
Environmental Fate Rate Constants, k, and Half-Lives, tₚₜ:
Half-Lives in the Environment:
14.1.4.24 2-Chlorosyringaldehyde

Common Name: 2-Chlorosyringaldehyde
Synonym:
Chemical Name: 2-chlorosyringaldehyde
CAS Registry No: 76341-69-0
Molecular Formula: C₉H₉ClO₄, C₆H(OH)Cl(CHO)(OCH₃)₂
Molecular Weight: 216.619
Melting Point (°C):
196–197 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
6.80 (Varhaníčková et al 1995)
Molar Volume (cm³/mol):
209.1 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
77.7 (Lei et al. 1999)
Enthalpy of Sublimation, ∆Hₛᵤₗ (kJ/mol):
Enthalpy of Fusion, ∆Hₕₚ (kJ/mol):
Entropy of Fusion, ∆Sₕₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕₚ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
33 (at pH 5.30, shake flask-HPLC/UV, Varhaníčková et al 1995)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.079 (supercooled liquid Pᵥ, GC-RT correlation; Lei et al. 1999)
log (Pᵥ/Pa) = –4058/(T/K) – 12.51, (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.069 (calculated-Pᵥ/Cᵥ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kᵥₒₜₐₜ:
1.81 (quoted, NCASI 1992)
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kₒᵢ:
0.62 (estimated-Kᵥₒₜₐₜ, NCASI 1992)
Sorption Partition Coefficient, log Kₒₑ:
Environmental Fate Rate Constants, k, and Half-Lives, tᵢ:
Half-Lives in the Environment:
14.1.4.25 2,6-Dichlorosyringaldehyde

Common Name: 2,6-Dichlorosyringaldehyde
Synonym:
Chemical Name:
CAS Registry No: 76330-06-8
Molecular Formula: C₉H₈Cl₂O₄, C₆(OH)Cl₂(CHO)(OCH₃)₂
Molecular Weight: 251.064
Melting Point (°C):
195.6 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm³):
Acid Dissociation Constant, pKₐ:
Molar Volume (cm³/mol):
230.0 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
82.2 (Lei et al. 1999)
Enthalpy of Sublimation, ΔHₛₘₜ (kJ/mol):
Enthalpy of Fusion, ΔH₉ₜₖ (kJ/mol):
Entropy of Fusion, ΔS₉ₜₖ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS₉ₜₖ = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
26.0 (at pH 4.60, shake flask-HPLC/UV, Varhaníčková et al. 1995)
Vapor Pressure (Pa at 25°C):
0.025 (supercooled liquid Pₛ, GC-RT correlation; Lei et al. 1999)
log (Pₛ/Pa) = −4293/(T/K) − 12.79, (GC-RT correlation, Lei et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
0.0037 (calculated-Pₛ/Cₛ, Lei et al. 1999)
Octanol/Water Partition Coefficient, log Kₒ₍ₘ:
2.52 (quoted, NCASI 1992)
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kₒ:
1.19 (estimated-Kₒₘ, NCASI 1992)
Sorption Partition Coefficient, log Kₒₑ:
Environmental Fate Rate Constants, k, and Half-Lives, t½:
Half-Lives in the Environment:
### 14.2 SUMMARY TABLES AND QSPR PLOTS

#### TABLE 14.2.1
Summary of physical properties of phenolic compounds

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<td>94.111</td>
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<td>C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt;(CH&lt;sub&gt;3&lt;/sub&gt;)OH</td>
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<td>72.5</td>
<td>216.9</td>
<td>0.342</td>
<td>147.8</td>
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<td>170.0</td>
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<td>232.6</td>
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<td>94.5</td>
<td>233</td>
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<td>170.0</td>
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(Continued)
### TABLE 14.2.1 (Continued)

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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>
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**Chlorophenols:**

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<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>
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<td>$C_{6}H_{4}Cl_2O$</td>
<td>163.001</td>
<td>59</td>
<td>211</td>
<td>0.464</td>
<td>145.2</td>
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<td>68</td>
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<td>233</td>
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<td>197.446</td>
<td>83.5</td>
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<td>4901-51-3</td>
<td>C₆H₃Cl₄O</td>
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<td>70</td>
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<td>Pentachlorophenol</td>
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<td>C₆H₂Cl₅O</td>
<td>266.336</td>
<td>174</td>
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<td>4-Chloro-α-m-cresol</td>
<td>59–50–7</td>
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<td>142.583</td>
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<td>C₆H₄N₂O₅</td>
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<td>Catechol (1,2-Dihydroxybenzenene)</td>
<td>120-80-9</td>
<td>C₆H₄(OH)₂</td>
<td>110.111</td>
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<td>C₆H₅Cl(OH)₂</td>
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<td>116–117</td>
<td>152.6</td>
<td>7.78</td>
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<td>C₆H₅Cl(OH)₂</td>
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<td>C₆H₅Cl(OH)₂</td>
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<td>194.4</td>
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<td>Resorcinol (1,3-Dihydroxybenzene)</td>
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<td>C₆H₄(OH)₂</td>
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<td>109.4</td>
<td>276.5</td>
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<td>Hydroquinone</td>
<td>123-31-9</td>
<td>C₆H₄(OH)₂</td>
<td>110.111</td>
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<td>32</td>
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<td>124.138</td>
<td>&lt; B17</td>
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<td>4-Methoxyphenol</td>
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<td>243</td>
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<td>5-Chloroguaiacol</td>
<td>3753-23-5</td>
<td>C₆H₅ClO₂</td>
<td>158.582</td>
<td>34–35</td>
<td>155.6</td>
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<td>4,5-Dichloroguaiacol</td>
<td>2460-49-3</td>
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<td>69–79</td>
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<td>63–64</td>
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<td>Tetrachloroguaiacol</td>
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<td>C₆H₅ClO₂</td>
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<td>C₆H₅ClO₃</td>
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<td>171–172</td>
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<td>Molecular formula</td>
<td>Molecular weight, MW g/mol</td>
<td>m.p. °C</td>
<td>b.p. °C</td>
<td>Fugacity ratio, F at 25°C*</td>
<td>Molar volume, ( V_m ) cm³/mol</td>
</tr>
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<td>5,6-Dichlorovanillin</td>
<td>18113–22–9</td>
<td>( \text{C}_8\text{H}_6\text{Cl}_2\text{O}_3 )</td>
<td>221.038</td>
<td>198–199</td>
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<td>Syringol (2,6-Dimethoxyphenol)</td>
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<td>( \text{C}<em>8\text{H}</em>{10}\text{O}_3 )</td>
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<td>18113–22–9</td>
<td>( \text{C}_8\text{H}_9\text{ClO}_3 )</td>
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<td>( \text{C}_8\text{H}_8\text{Cl}_2\text{O}_3 )</td>
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<td>Trichlorosyringol</td>
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<td>257.499</td>
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<td>2-Chlorosyringaldehyde</td>
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<td>( \text{C}_9\text{H}_9\text{ClO}_4 )</td>
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* Assuming \( \Delta S_{\text{ fus }} = 56 \text{ J/mol K.} \)
### TABLE 14.2.2
Summary of selected physical-chemical properties of phenolic compounds at 25°C

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<th>Compound</th>
<th>Vapor pressure</th>
<th>Selected properties</th>
<th>Henry's law constant</th>
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<td>Pₛ/Pa</td>
<td>Pᵥ/Pa</td>
<td>S/(g/m^3)</td>
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<td>p-Cresol (4-Methylphenol)</td>
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(Continued)
TABLE 14.2.2 (Continued)

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<th>Solubility</th>
<th>Henry's law constant</th>
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<td>( S/\text{g/m}^3 )</td>
<td>( C^3/\text{mol/m}^3 )</td>
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<td>12.6</td>
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<td>2,4,5-Trichlorophenol</td>
<td>2.5</td>
<td>6.76</td>
<td>948</td>
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<td>2,4,6-Trichlorophenol</td>
<td>1.25</td>
<td>3.44</td>
<td>434</td>
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<td>3,4,5-Trichlorophenol</td>
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<td>Phenolic Compounds</td>
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<td>---</td>
<td>---</td>
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<tr>
<td>2,3,4,5-Tetrachlorophenol</td>
<td>0.1</td>
<td>0.79</td>
<td>166</td>
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<tr>
<td>2,3,4,6-Tetrachlorophenol</td>
<td>0.28</td>
<td>0.78</td>
<td>183</td>
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<td>2,3,5,6-Tetrachlorophenol</td>
<td>0.1</td>
<td>0.78</td>
<td>100</td>
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<tr>
<td>Pentachlorophenol</td>
<td>4.15×10⁻³</td>
<td>0.12</td>
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**Nitrophenols:**

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<tr>
<th>Nitrophenol</th>
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<th></th>
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<th></th>
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<tbody>
<tr>
<td>2-Nitrophenol</td>
<td>20</td>
<td>1080</td>
<td>7.764</td>
<td>12.15</td>
<td>1.8</td>
<td>1.646</td>
</tr>
<tr>
<td>3-Nitrophenol</td>
<td>11550</td>
<td>83.03</td>
<td>421.5</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-Nitrophenol</td>
<td>13500</td>
<td>97.05</td>
<td>718.9</td>
<td>1.91</td>
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<td></td>
</tr>
<tr>
<td>2,4-Dinitrophenol</td>
<td>335</td>
<td>1.820</td>
<td>13.78</td>
<td>1.67</td>
<td></td>
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<tr>
<td>2,4,6-Trinitrophenol (Picric acid)</td>
<td>13750</td>
<td>60.02</td>
<td>540.7</td>
<td>1.33</td>
<td></td>
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<tr>
<td>4,6-Dinitro-α-cresol</td>
<td>222</td>
<td>1.120</td>
<td>4.500</td>
<td>2.12</td>
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**Dihydroxybenzenes, methoxyphenols and chloroguaiacols:**

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<th></th>
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<tbody>
<tr>
<td>Catechol (1,2-Dihydroxybenzene)</td>
<td>0.0118</td>
<td>0.079</td>
<td>110000</td>
<td>999.0</td>
<td>6705</td>
<td>0.80</td>
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<tr>
<td>Hydroquinone (1,4-Dihydroxybenzene)</td>
<td>2.55×10⁻³</td>
<td>0.071</td>
<td>70000</td>
<td>635.7</td>
<td>17758</td>
<td>0.59</td>
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<tr>
<td>2-Methoxyphenol (Guaiacol)</td>
<td>20.825</td>
<td>24.4</td>
<td>24800</td>
<td>199.8</td>
<td>233.9</td>
<td>1.33</td>
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<tr>
<td>3-Methoxyphenol</td>
<td>67800</td>
<td>546.2</td>
<td>546.2</td>
<td>1.58</td>
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<td>4-Methoxyphenol</td>
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<td>157.1</td>
<td>323.9</td>
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<td>4-Chloroguaiacol</td>
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<td>5-Chloroguaiacol</td>
<td>3960</td>
<td>24.97</td>
<td>30.94</td>
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<tr>
<td>4,5-Dichloroguaiacol</td>
<td>0.570</td>
<td>1.72</td>
<td>575</td>
<td>2.98</td>
<td>9.000</td>
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<td>4,6-Dichloroguaiacol</td>
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<td>3.668</td>
<td>8.754</td>
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<td>3,4,5-Trichloroguaiacol</td>
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<td>0.64</td>
<td>310</td>
<td>1.363</td>
<td>5.344</td>
<td>3.77</td>
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<td>4,5,6-Trichloroguaiacol</td>
<td>0.032</td>
<td>0.23</td>
<td>54</td>
<td>0.2374</td>
<td>1.733</td>
<td>3.74</td>
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<tr>
<td>Tetrachloroguaiacol</td>
<td>0.016</td>
<td>0.14</td>
<td>26</td>
<td>0.0993</td>
<td>0.8785</td>
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### TABLE 14.2.3
Suggested half-life classes for phenolic compounds in various environmental compartments at 25°C

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<th>Compound</th>
<th>Air class</th>
<th>Water class</th>
<th>Soil class</th>
<th>Sediment class</th>
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<td>3</td>
<td>4</td>
<td>5</td>
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<tr>
<td>o-Cresol</td>
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<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>p-Cresol</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>2,4-Dimethylphenol</td>
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<td>3</td>
<td>4</td>
<td>5</td>
</tr>
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<td>Chlorophenols:</td>
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<td></td>
<td></td>
</tr>
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<td>3</td>
<td>3</td>
<td>5</td>
<td>6</td>
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<tr>
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<td>4</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>2,4,6-Trichlorophenol</td>
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<td>4</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
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<td>5</td>
<td>6</td>
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<td>3</td>
<td>3</td>
<td>5</td>
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<td>4-Nitrophenol</td>
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<td>3</td>
<td>5</td>
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<td>4</td>
<td>6</td>
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<td>4</td>
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<td>4,6-Dinitro-o-cresol</td>
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<td>4</td>
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<td>Dihydroxybenzenes, methoxyphenols and chloroguaiacols:</td>
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<tr>
<td>Catechol</td>
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<td>5</td>
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<tr>
<td>2-Methoxyphenol (Guaiacol)</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>Tetrachloroguaiacol</td>
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<td>4</td>
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where,

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<th>Class</th>
<th>Mean half-life (hours)</th>
<th>Range (hours)</th>
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<tr>
<td>1</td>
<td>5</td>
<td>&lt; 10</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>
</tr>
<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>
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</table>
FIGURE 14.2.1  Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

FIGURE 14.2.2  Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.
FIGURE 14.2.3 Octanol-water partition coefficient versus Le Bas molar volume for phenolic compounds.

FIGURE 14.2.4 Henry's law constant versus Le Bas molar volume for phenolic compounds.
FIGURE 14.2.5  Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for phenolic compounds.
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3012 Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals


Phenolic Compounds


# 15 Esters

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<td>Tris(2-ethylhexyl) phosphate (TEHP)</td>
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<td>15.1.4.4</td>
<td>Trihaloalkyl phosphates</td>
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15.1 LIST OF CHEMICALS AND DATA COMPILATIONS

15.1.1 ALIPHATIC ESTERS

15.1.1.1 Methyl formate

Common Name: Methyl formate
Synonym: formic acid methyl ester, methyl methanoate
Chemical Name: methyl formate
CAS Registry No: 107-31-3
Molecular Formula: C₂H₄O₂, HCOOCH₃
Molecular Weight: 60.052

Melting Point (°C):
-99.0 (Weast 1982–83; Dean 1985; Lide 2003)
Boiling Point (°C):
31.7 (Lide 2003)

Density (g/cm³ at 20°C):
0.9742 (Weast 1982–83)
0.9742, 0.9664 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
62.8 (exptl. at normal bp, Lee et al. 1972)
61.6 (20°C, calculated-density)
62.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
30.59; 29.72 (25°C; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔHᶠus (kJ/mol):
7.75 (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):
230000 (USEPA 1975; quoted, Howard 1993)
304000 (20°C, Verschueren 1983)
230000 (Dean 1985; Riddick et al. 1986)
23800 (solubility data compilation, 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):
83260* (isoteniscope method, measured range 21–31.7°C, Nelson 1928)
log (P/mmHg) = 7.2202 – 1320.8/(T/K); temp range 21–31.7°C, Nelson 1928)
53329* (16°C, summary of literature data, temp range –74.2 to 213°C, Stull 1947)
log (P/mmHg) = [-0.2185 × 7027.8/(T/K)] + 7.852144; temp range –74.2 to 213°C (Antoine eq., Weast 1972–73)
63980, 93310 (20°C, 30°C, Verschueren 1983)
80840 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 2.11093 – 1.573/(–17.263 + t/°C), temp range: 21–31.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
83440 (calculated-Antoine eq., Dean 1985)
log (P/mmHg) = 3.207 – 3.02/(–11.9 + t/°C), temp range: 21–32°C (Antoine eq., Dean 1985, 1992)
78060 (selected lit., Riddick et al. 1986)
log (P/kPa) = 6.29529 – 1125.2/(174.2 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
78600 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P$_L$/kPa) = 6.225693 – 1088.955/(–46.675 + T/K); temp range 279–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P$_L$/kPa) = 6.39684 – 1196.323/(–32.629 + T/K); temp range 305–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)
78070 (Daubert & Danner 1989)
log (P/mmHg) = 28.9576 – 2.3582 × 10$^3$/T/K –7.4848·log(T/K) + 7.4384 × 10$^{-10}$·(T/K) + 2.7013 × 10$^{-6}$·(T/K)$^2$, temp range 174–487 K (vapor pressure eq., Yaws 1994)
114881 (35°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry’s Law Constant (Pa·m$^3$/mol at 25°C):
22.61 (exptl., Hine & Mookerjee 1975)
20.15, 17.96 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
15.64 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
26.02 (calculated-P/C, Hoff et al. 1993)

Octanol/Water Partition Coefficient, log $K_{ow}$:
−0.010 (calculated-intrinsic molar volume $V_I$ and solvatochromic parameters, Leahy 1986)
−0.264 (estimated, Howard 1993)
0.03 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log $BCF$:
−0.222 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, log $K_{OC}$:
0.699 (soil, estimated-S, Lyman et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: based on Henry’s law constant, $t_{1/2} = 5.3$ h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

\[ k_{OH} = (2.27 \pm 0.34) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a, quoted, Atkinson 1989)} \]

\[ k_{OH}(\text{calc}) = 0.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1996)} \]

Hydrolysis: aqueous base-catalyzed hydrolysis $k = 36.6$ M$^{-1}$ s$^{-1}$ at 25°C corresponds to $t_{1/2} = 21.9$ d, 2.19 d, 9.1 h and 0.91 h at respective pHs of 6, 7, 8, and 9 (Mabey & Mill 1978; quoted, Howard 1993)

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

Half-Lives in the Environment:
Air: estimated $t_{1/2} = 74$ d, based on experimental reaction rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere at 23°C (Atkinson 1989; quoted, Howard 1993).
TABLE 15.1.1.1.1
Reported vapor pressures of methyl formate at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Nelson 1928</th>
<th>Stull 1947</th>
</tr>
</thead>
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<tr>
<td>isotonoscope</td>
<td>summary of literature data</td>
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<td>P/Pa</td>
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<td>26.6</td>
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<td>b.p/°C</td>
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<td>eq. 1</td>
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<td>A</td>
<td>7.2203</td>
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<tr>
<td>B</td>
<td>1329.8</td>
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</tbody>
</table>

FIGURE 15.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methyl formate.
15.1.1.2 Ethyl formate

Common Name: Ethyl formate
Synonym: ethyl methanoate, formic acid ethyl ester
Chemical Name: ethyl formate
CAS Registry No: 109-94-4
Molecular Formula: C₃H₆O₂, HCOOCH₂CH₃
Molecular Weight: 74.079

Melting Point (°C): ~79.6 (Lide 2003)
Boiling Point (°C): 54.4 (Lide 2003)
Density (g/cm³ at 20°C): 0.9168 (Weast 1982–83), 0.9220, 0.9153 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol): 80.8 (20°C, calculated-density, Stephenson & Malanowski 1987), 86.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pKₐ:

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
31.64; 29.94 (25°C; bp, Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
9.205 (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):
88250 (Seidell 1941), 93260 (estimated, McGowan 1954), 52440 (Deno & Berkheimer 1960), 118000 (Verschueren 1983; Riddick et al. 1986), 117000 (Dean 1985)

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

34530* (25.4°C, isoteniscopie method, measured range 25.4–55.4°C, Nelson 1928)
\[ \log (P/\text{mmHg}) = 7.8457 - 1621.2/(T/K); \] temp range 25.4–55.4°C (Nelson 1928)

33050* (interpolated-regression of tabulated data, temp range –60.5 to 54.3°C, Stull 1947)

\[ \log (P/\text{mmHg}) = \left[ -0.2185 \times 7511.7/(T/K) \right] + 7.842747; \] temp range –60.5 to 225°C (Antoine eq., Weast 1972–73)

25590, 39990 (20°C, 30°C, Verschueren 1983)

30840, 32610 (23.7°C, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{mmHg}) = 6.13263 - 1123.305/(218.177 + t/°C); \] temp range 3.89–53.56°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

32540 (interpolated-Antoine eq., Dean 1985)
\[ \log (P/\text{mmHg}) = 7.0090 - 1123.94/(218.2 + t/°C); \] temp range 4–54°C (Antoine eq., Dean 1985, 1992)

32370 (selected, Riddick et al. 1986)

33070 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\[ \log (P_P/\text{kPa}) = 6.1384 - 1151.08/[–48.94 + (T/K)]; \] temp range: 213–336 K (Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log (P_P/\text{kPa}) = 6.4206 - 1326.4/[–26.867 + (T/K)]; \] temp range: 327–498 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 29.9404 – 2.5263 × 10^3/(T/K) – 7.809·log(T/K) – 1.0111 × 10^{-9}·(T/K)^2;
temp range 194–508 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C):
28.46 (exptl., Hine & Mookerjee 1975)
27.18, 25.96 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
17.55 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
702.0 (calculated, Hoff et al. 1993)

Octanol/Water Partition Coefficient, log K_{ow}:
–0.38 (calculated, Iwasa et al. 1965)
0.23 (calculated, Hansch et al. 1968)
0.33 (Leo et al. 1971)
0.55 (calculated-intrinsic molar volume V_i and solvatochromic parameters, Leahy 1986)
0.26 (calculated-CLOGP, Müller & Klein 1992)

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

Biocconcentration 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 as indicated, *data at other temperatures see reference:
k_{OH} = (10.2 ± 1.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington
et al. 1988a; quoted, Atkinson 1989)
k_{OH} = 10.2 × 10^{-12} cm^3 molecule^{-1} s^{-1}; k(soln) = 6.5 × 10^{-13} cm^3 molecule^{-1} s^{-1} for reaction with OH radical
in aqueous solution (Wallington et al. 1988a)
k_{OH(calc)} = 1.17 × 10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:
Biodegradation:
Biotransformation:

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

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 15.1.1.2.1</th>
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<tbody>
<tr>
<td>Reported vapor pressures of ethyl formate at various temperatures and the coefficients for</td>
</tr>
<tr>
<td>the vapor pressure equations</td>
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</tbody>
</table>

log P = A – B/(T/K) \quad (1) \quad \ln P = A – B/(T/K) \quad (1a)
log P = A – B/(C + t/°C) \quad (2) \quad \ln P = A – B/(C + t/°C) \quad (2a)
log P = A – B/(C + T/K) \quad (3)
log P = A – B/(T/K) – C·log (T/K) \quad (4)

**Nelson 1928**

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<th>\text{t}/°C</th>
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<tr>
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**Stull 1947**

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<td>–60.5</td>
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**Mertl & Polak 1964**

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TABLE 15.1.1.2.1 (Continued)

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bp/°C  53.8  eq. 2 P/kPa

bp/°C  54.0

eq. 1 P/mmHg

A  7.8457  B  1123.305

B  1621.6  C  218.177

bp/°C  54.013

FIGURE 15.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl formate.
15.1.1.3 Propyl formate

Common Name: Propyl formate
Synonym: formic acid propyl ester, methanoic acid \( n \)-propyl ester, propyl methanoate
Chemical Name: \( n \)-propyl formate, propyl formate
CAS Registry No: 110-74-7
Molecular Formula: \( \text{C}_4\text{H}_8\text{O}_2, \text{HCOOCH}_2\text{CH}_2\text{CH}_3 \)
Molecular Weight: 88.10
Melting Point (°C): –92.9
Boiling Point (°C): 80.9
Density (g/cm\(^3\) at 20°C):
\( 0.9058 \) (Weast 1982–83)
\( 0.9006 \) (Dean 1985)
\( 0.9055, 0.8996 \) (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
\( 97.3 \) (20°C, calculated-density)
\( 110.8 \) (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK\(_a\): 37.49; 33.60 (25°C; bp, Riddick et al. 1986)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
\( 37.49; 33.60 \) (25°C; bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
\( 28445 \) (Seidell 1941)
\( 27230 \) (Deno & Berkheimer 1960)
\( 27300 \) (Hansch et al. 1968; quoted, Hine & Mookerjee 1975; Müller & Klein 1992)
\( 20500 \) (Dean 1985; 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):
\( 11759^* \) (26.2°C, isotoniscope method, measured range 26.2–82.3°C, Nelson 1928)
\( \log (P/\text{mmHg}) = 7.9925 – 1806.5/(T/K) \); temp range 26.2–82.3°C (Nelson 1928)
\( 10620^* \) (interpolated-regression of tabulated data, temp range –43 to 81.3°C Stull 1947)
\( \log (P/\text{mmHg}) = [-0.2185 \times 8208.1/(T/K)] + 7.891833; \) temp range –43 to 245°C (Antoine eq., Weast 1972–73)
\( 11010 \) (calculated-Antoine eq., Boublik et al. 1984)
\( \log (P/\text{Pa}) = 5.98912 – 1135.489/(204.518 + t/°C); \) temp range: 26.2–82.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
\( 10710 \) (extrapolated-Antoine eq., Dean 1985)
\( \log (P/\text{mmHg}) = 6.848 – 1127/(203 + t/°C); \) temp range: 26–82°C (Antoine eq., Dean 1985, 1992)
\( 11030 \) (quoted lit. average, Riddick et al. 1986)
\( \log (P/\text{kPa}) = 5.97008 – 1132.3/(204.8 + t/°C); \) temp range not specified (Antoine eq., Riddick et al. 1986)
\( 10810 \) (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\( \log (P/\text{kPa}) = 6.73268 – 1560.69/(–24.287 + T/K); \) temp range: 230–335 K (Antoine eq.-I, Stephenson & Malanowski 1987)
\( \log (P/\text{kPa}) = 6.2378 – 1301.3/(–46.767 + T/K); \) temp range: 354–518 K (Antoine eq.-II, Stephenson & Malanowski 1987)

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\[
\log (P/mmHg) = 28.6983 - 2.6926 \times 10^{3}/(T/K) - 7.2435\log(T/K) - 8.7226 \times 10^{-11}(T/K)^2;
\text{temp range 180–538 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa·m^3/mol at 25°C):
- 37.52 (exptl., Hine & Mookerjee 1975)
- 22.61 (calculated-MCI \(\chi\), Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log \(K_{ow}\):
- 0.73 (calculated, Hansch et al. 1968)
- 0.83 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979)
- 0.83 (recommended, Sangster 1989; 1993)
- 0.83 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \(K_{oa}\):
- 2.66 (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:
  \(k_{OH} = (2.38 \pm 2.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988; quoted, Atkinson 1989)
  \(k_{OH}(\text{calc}) = 1.87 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) (molecular orbital calculations, Klamt 1996)
- Hydrolysis:
- Biodegradation:
- Biotransformation:

Half-Lives in the Environment:

---

### TABLE 15.1.1.3.1

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

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FIGURE 15.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for n-propyl formate.
15.1.1.4 Methyl acetate

Common Name: Methyl acetate
Synonym: acetic acid methyl ester, ethanoic acid methyl ester, methyl ethanoate
Chemical Name: methyl acetate
CAS Registry No: 79-20-9
Molecular Formula: C₃H₆O₂, CH₃COOCH₃
Molecular Weight: 74.079
Melting Point (°C): –98.25 (Lide 2003)
Boiling Point (°C): 56.89 (Lide 2003)
Density (g/cm³ at 20°C):
0.9330 (Weast 1982–83)
0.9342 (Dean 1985)
0.9342, 0.9279 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
79.3 (20°C, calculated-density)
84.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
22.50 (pKₐ, Riddick et al. 1986)
Enthalpy of Vaporization, ΔHV (kJ/mol):
32.30, 30.33 (25°C; bp, Riddick et al. 1986)
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):
243730 (20°C, shake flask-turbidity, Fühner 1924)
294920 (estimated, McGowan 1954)
243500 (20°C, Stephen & Stephen 1963)
240000, 319000 (20°C, Verschueren 1983)
240000 (Dean 1985)
245000 (20°C, 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):
27980* (interpolated-regression of tabulated data, –52 to 57.8°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 7732.8/(T/K)] + 7.938782; temp range –57.2 to 225°C (Antoine eq., Weast 1972–73)
28830* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
log (P/kPa) = 6.24410 – 1183.700/(223.115 + t/°C); temp range 259.6–351.3 K (Antoine eq. from reported exptl. data, Boublik et al. 1984)
31330 (Verschueren 1983)
28830 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.25449 – 1189.608/(223.115 + t/°C); temp range –13.58 to 78.12°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.19357 – 1159.358/(219.913 + t/°C); temp range 1.76–55.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
28200 (calculated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.0652 – 1157.63/(219.73 + t/°C); temp range: 1–56°C (Antoine eq., Dean 1985, 1992)
28828 (lit. average, Riddick et al. 1986)
log (P/kPa) = 6.24410 – 1183.70/(222.414 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 6.190152 – 1157.622/(–53.426 + T/K); temp range 274–331 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.18771 – 1156.219/(–53.589 + T/K); temp range: 274–331 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 33.7235 – 2.7204 × 10³/(T/K) – 9.1182·log(T/K) – 9.4316 × 10⁻¹¹·(T/K)²; temp range 175–507 K (vapor pressure eq., Yaws 1994)

53808 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

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

9.190 (volatility-partial pressure, Butler & Ramchandani 1935)
11.65 (volatility-partial pressure-GC, Buttery et al. 1969)
8.795 (exptl., Hine & Mookerjee 1975)
13.06 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 39.2 kJ/mol, Kieckbusch & King 1979)
9.210, 25.96 (quoted, calculated-MCI χ, Nirmalkhankand & Speece 1988)
9.80 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log Kₐw = 4.590 – 2048/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log Kₐw:

0.18 (shake flask-CR, Collander 1951; quoted, Hansch & Leo 1979; Hansch & Leo 1985)
0.23 (calculated, Hansch et al. 1968)
0.70 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.18 (recommended, Sangster 1989, 1993)
0.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log Kₐα:

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

Bioconcentration Factor, log BCF:

–0.224 (calculated-S, Lyman et al. 1982)
–0.092 (calculated-Kₐw, Lyman et al. 1982)

Sorption Partition Coefficient, log Kₐc:

0.681 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
1.474 (soil, calculated-Kₐw, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t₀:

Volatilization: based on calculated Henry’s law constant, t₀ = 9.1 h from a model river of 1 m deep flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k₂OH for reaction with OH radical, k₂NO3 with NO₃ radical and k₂O₃ with O₃, or as indicated, *data at other temperatures see reference: photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

k₂OH = (1.1 ± 0.03) × 10⁻¹⁰ dm³ mol⁻¹ s⁻¹ or (1.7 ± 0.5) × 10⁻¹⁵ cm³ molecule⁻¹ s⁻¹ at 292 K using relative rate technique for n-butane (Campbell & Parkinson 1978)

k₂OH(exptl) = (1.3 – 3.41) × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988a,b; quoted, Howard 1993)

k₂OH(calc) = 1.9 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, k₂OH(obs.) = 1.7 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1985)
k_{OH}(calc) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{OH}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \ (\text{SAR structure-activity relationship, Atkinson 1987})

k_{OH} = (3.41 \pm 0.29) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K} \ (\text{absolute rate, flash photolysis-resonance fluorescence, Wallington 1988a})

k_{OH} = 3.41 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \ ; \ k(\text{soln}) = 2.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)}

k_{OH}(calc) = 6.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \ (\text{molecular orbital calculations, Klamt 1996})

Hydrolysis: alkaline hydrolysis rate constant k = 0.182 M^{-1} \text{ s}^{-1} \text{ at } 25^\circ \text{C} \text{ in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).}

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

Half-Lives in the Environment:
Air: photooxidation t_\frac{1}{2} = 2.4–24 \text{ h} \text{ 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); atmospheric t_\frac{1}{2} = 47–94 \text{ d}, based on exptl. rate constants for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988; quoted, Howard 1993)).

Surface water:
Groundwater:
Sediment:
Soil:
Biota:

**TABLE 15.1.1.4.1**

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

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<th>Temperature (°C)</th>
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**FIGURE 15.1.1.4.1** Logarithm of vapor pressure versus reciprocal temperature for methyl acetate.

b.p. = 56.87 °C
15.1.1.5 Vinyl acetate

Common Name: Vinyl acetate
Synonym: ethanoic acid ester, ethenyl acetate, ethenyl ethanoate
Chemical Name: ethenyl acetate, vinyl acetate
CAS Registry No: 108-05-4
Molecular Formula: C4H6O2, CH3COOCH=CH2
Molecular Weight: 86.090
Melting Point (°C):
Boiling Point (°C):
   72.8 (Lide 2003)
Density (g/cm³ at 20°C):
   0.9317 (Weast 1982–83)
Molar Volume (cm³/mol):
   92.2 (20°C, calculated-density, Stephenson & Malanowski 1987)
   101.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ∆HV (kJ/mol):
   37.2, 34.35 (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):
   19722 (Deno & Berkheimer 1960)
   25000 (Verschueren 1983)
   20000 (Dean 1985)
   20000 (20°C, 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):
   14454* (interpolated-regression of tabulated data, temp range –48 to 72.5°C, Stull 1947)
   84406* (67°C, vapor-liquid equilibrium data, measured range 67–82°C, Swamy & Van Winkle 1965)
   15300 (interpolated-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 7.17023 – 1766.918/(269.951 + t/°C); temp range: 67–82°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   log (P/kPa) = 6.3363 – 1296.847/(226.731 + t/°C); temp range: 21.83–72.04°C (Antoine eq. from reported exptl. data, Dean 1985, 1992)
   15300 (interpolated-Antoine eq., Dean 1985, 1992)
   log (P/mmHg) = 7.2101 – 1296.13/(226.66 + t/°C); temp range: 22–72°C (Antoine eq., Dean 1985, 1992)
   14100 (quoted lit. average, Riddick et al. 1986)
   log (P/kPa) = 7.216 – 1798.4/(T/K); temp range: not specified (Antoine eq., Riddick et al. 1986)
   15340, 15305 (interpolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
   log (P/kPa) = 6.3799 – 1320.2716/(–43.96 + T/K); temp range: 293–346 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P/kPa) = 6.34264 – 1300.315/(–46.041 + T/K); temp range 294–346 K (Antoine eq.-II, Stephenson & Malanowski 1987)
   11320 (20°C, quoted, Howard 1989)
log \( \frac{\text{P/mmHg}}{\text{T/K}} = 12.722 - 2.177 \times 10^3 \frac{\text{T/K}}{\text{T/K}} - 91.458 \log \frac{\text{T/K}}{\text{T/K}} - 4.5688 \times 10^{-3} \frac{\text{T/K}}{\text{T/K}} + 2.9673 \times 10^{-6} \frac{\text{T/K}}{\text{T/K}}^2 \); temp range 180–524 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
48.74 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
0.60 (shake flask, Fujisawa & Masuhara 1980)
0.21 (calculated-HPLC-RT, Fujisawa & Masuhara 1981)
0.73 (recommended, Sangster 1989, 1993)
0.73 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.32–0.37 (estimated-\( K_{\text{OW}} \), Howard 1989)

Sorption Partition Coefficient, log \( K_{\text{OC}} \):
1.28–1.77 (estimated-\( K_{\text{OW}} \), Howard 1989)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\text{1/2} \):
Volatilization: estimated \( t_{\text{1/2}} = 4.4 \text{ h} \) from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and \( t_{\text{1/2}} = 2.2 \text{ d} \) from an environmental pond (Howard 1989).
Photolysis:
Oxidation: \( t_{\text{1/2}} = 13 \text{ and } 8 \text{ d} \) for reactions with OH radical and singlet oxygen in sunlit natural water (Howard 1989).
Hydrolysis: overall rate constant \( k_h = 1.10 \times 10^{-6} \text{ s}^{-1} \) with \( t_{\text{1/2}} = 7.3 \text{ d} \) at 25°C and pH 7 (Mabey & Mill 1978) degradation \( t_{\text{1/2}} = 7.3 \text{ d} \) at 25°C and pH 7, the hydrolysis rate will increase as the pH increases (Howard 1989).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_{\text{i}} \)) and Elimination (\( k_{\text{e}} \)) Rate Constants:

Half-Lives in the Environment:
Air: estimated \( t_{\text{1/2}} = 12 \text{ h} \) with photochemically produced hydroxyl radical in an average atmosphere (Howard 1989).
Surface water: hydrolysis degradation \( t_{\text{1/2}} = 7.3 \text{ days} \) at 25°C and pH 7; \( t_{\text{1/2}} = 13 \text{ and } 8 \text{ d} \) for reactions with hydroxyl radical and singlet oxygen, respectively, in natural water (Howard 1989).
Groundwater:
Sediment:
Soil:
Biota:
TABLE 15.1.1.5.1
Reported vapor pressures of vinyl acetate at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947

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mp/°C –73

Capkova & Fried 1963

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eq. 2 P/kPa

A 6.33630
B 1296.847
C 226.731
bp/°C 71.731

Swamy & Van Winkle 1965

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V–L equil. data

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b.p. = 72.8 °C

FIGURE 15.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for vinyl acetate.
15.1.1.6 Ethyl acetate

Common Name: Ethyl acetate
Synonym: acetic acid ethyl ester, acetic ether, ethanoic acid ester, ethyl ethanoate  
Chemical Name: \( n \)-ethyl acetate, ethyl acetate
CAS Registry No: 141-78-6  
Molecular Formula: \( \text{C}_4\text{H}_8\text{O}_2 \), \( \text{CH}_3\text{COOCH}_2\text{CH}_3 \)  
Molecular Weight: 88.106  
Melting Point (°C):  
\(-83.8\) (Lide 2003)
Boiling Point (°C):  
\(77.11\) (Lide 2003)
Density (g/cm³ at 20°C):  
\(0.9003\) (Weast 1982–83)
\(0.9006, 0.8946\) (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):  
\(106.0\) (exptl. at normal bp, Lee et al. 1972)
\(97.8\) (20°C, calculated-density)
\(108.6\) (calculated-Le Bas method at normal boiling point)
Dissociation Constant:  
\(22.83\) (pKs, Riddick et al. 1986)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):  
\(35.62, 31.97\) (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):  
\(10.50\) (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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):  
\(64408\) (20°C, shake flask-turbidity, Fühner 1924)
\(85300\) (20°C, synthetic method, Jones 1929)
\(78720\) (shake flask-centrifuge, Booth & Everson 1948)
\(80100^*\) (turbidimetric method, measured range 20–40°C, Altshuller & Everson 1953)
\(80400^*\) (average, Altshuller & Everson 1953)
\(79780\) (shake flask-interferometry, Donahue & Bartell 1952)
\(69990\) (estimated, McGowan 1954)
\(82220\) (Deno & Berkheimer 1960)
\(80350\) (shake flask-UV, Hansch et al. 1968)
\(63960\) (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
\(82500, 74000\) (20°C, 35°C, literature average, Verschueren 1983)
\(80000\) (shake flask-HPLC, Banerjee 1984)
\(97000\) (Dean 1985)
\(95000\) (shake flask-radiometric method, Lo et al. 1986)
\(80800\) (lit. average, Riddick et al. 1986)
\(77900^*\) (20.2°C, shake flask-GC/TC, measured range 0–70°C, Stephenson & Stuart 1986)
\(73700\) (solubility data compilation, 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):  
\(13330^*, 11860\) (27.0°C, interpolated-regression of tabulated data, temp range –43.4 to 78.1°C, Stull 1947)
\(\log (\text{P/mmHg}) = 7.30588 – 1357.7/(230 + t^\circ\text{C})\) (Antoine eq., Dreisbach & Martin 1949)
13155* (25.86°C, temp range 15.58–75.830°C, Mertl & Polak 1964; quoted, Boublik et al. 1984)
log (P/mmHg) = [–0.2185 × 8301.1/(T/K)] + 8.001170; temp range –43.4 to 235°C (Antoine eq., Weast 1972–73)
12600* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
log (P/kPa) = 6.18799 – 1224.673/(215.712 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
12620 (calculated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.10179 – 1244.95/(217.88 + t/°C) temp range 15–76°C (Antoine eq., Yaws 1994)
25078 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry’s Law Constant (Pa·m3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
13.42 (partial pressure, Butler & Ramchandani 1935)
17.78 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
13.62 (exptl., Hine & Mookerjee 1975)
15.64, 13.94 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
17.20 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ∆H = 41.4 kJ/mol, Kieckbusch & King 1979)
13.62, 24.22 (quoted, calculated-MCI χ, Nimalakhandan & Speece 1988)
41.72* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
ln (1/KAW) = –7.28 + 3563/(T/K), temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
13.62, 6.23 (quoted, calculated-molecular structure, Russell et al. 1992)
11.33 (calculated, Hoff et al. 1993)
13.51 (solid-phase microextraction SPME-GC, Bartelt 1997)
12.72 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K\text{AW} = 5.095 – 2163/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K\text{OW}:
0.66 (shake flask-chemical reaction CR, Collander 1951)
0.73 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1969, 1971; Hansch & Leo 1979)
0.73 (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979)
0.65, 0.66 (calculated-τ substituent const.; calculated-fragment const., Rekker 1977)
0.70 (exptl., Valvani et al. 1981; quoted, Amidon & Williams 1982)
0.53 (calculated-activity coeff. γ, Wasik et al. 1981)
0.68 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
1.02 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.73 (recommended, Sangster 1989, 1993)
0.73 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

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

Bioconcentration Factor, log $BCF$:

4.13 (algae $Chlorella fusca$, wet wt. basis, Geyer et al. 1984)
0.70 (algae $Chlorella fusca$, calculated-$K_{OW}$, Geyer et al. 1984)
1.48 (golden ide, Freitag et al. 1985)
4.13 (algae, Freitag et al. 1985)
3.52 (activated sludge, Freitag et al. 1985)

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

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

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

Volatilization: using Henry’s law constant, $t_{1/2}$ ~ 10.1 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; quoted, Howard 1990).

Photolysis: rate constant $k = 6.8 \times 10^{-4} \text{ h}^{-1}$ to 2.21 $\times 10^{-3} \text{ h}^{-1}$ with $\text{H}_2\text{O}_2$ under photolysis at 25°C in F-113 solution and with $\text{HO}^-$ in the gas (Dilling et al. 1988).

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

photooxidation $t_{1/2} = 2.75–110 \text{ yr}$ in water, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 2.4–24 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.16 \pm 0.13) \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 292 K using relative rate technique for n-butane (Campbell & Parkinson 1978)

$k_{OH}(calc) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(obs.) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(calc) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(obs.) = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (15.1 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 296–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted Atkinson 1989)

$k_{OH} = 1.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(calc) = 1.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.110 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

overall rate constant $k_{OH} = 1.10 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 2.0 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 2.0 \text{ yr}$, based on measured rate constants for acid and base catalyzed and neutral hydrolysis at pH 7 and 20°C (Mabey & Mill 1978; quoted, Howard 1990; Howard et al. 1991; Kollig 1993)

$t_{1/2} = 9.5 \times 10^7 \text{ d}$ at pH 2, $t_{1/2} = 740 \text{ d}$ at pH 7 and $t_{1/2} = 97000 \text{ d}$ at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 24–168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Price et al. 1974; selected, 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)

$t_{1/2}(aerobic) = 1 \text{ d}$, $t_{1/2}(anaerobic) = 4 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.75–110 \text{ yr}$, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);
$t_{1/2} = 2.4–24\ h$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976); 
photodecomposition $t_{1/2} = 14.6\ h$ under simulated atmospheric conditions, with NO (Dilling et al. 1976) photooxidation $t_{1/2} = 35.3–353\ h$, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991); 
calculated lifetimes of 6.9 d and 10 yr for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000). 
Surface water: $t_{1/2} = 24–168\ h$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biodegradation $t_{1/2}$ (aerobic) = 1 d, $t_{1/2}$ (anaerobic) = 4 d; hydrolysis $t_{1/2} = 9.5 \times 10^7\ d$ at pH 2, $t_{1/2} = 740\ d$ at pH 7 and $t_{1/2} = 97000\ d$ at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)
Groundwater: $t_{1/2} = 24–168\ h$, 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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FIGURE 15.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl acetate.

TABLE 15.1.1.6.2
Reported vapor pressures of ethyl acetate at various temperatures and the coefficients for the vapor pressure equations

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

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(Continued)
TABLE 15.1.1.6.2 (Continued)

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<td>B</td>
<td>1245.172</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>217.904</td>
<td></td>
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<tr>
<td>bp</td>
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<td></td>
</tr>
</tbody>
</table>

Stull 1947
Mertl & Polak 1965
Ambrose et al. 1981

Comparative ebulliometry

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>eq. 3</td>
<td>P/kPa</td>
<td>A</td>
<td>6.18799</td>
</tr>
<tr>
<td>B</td>
<td>1224.673</td>
<td>Chebyshev polynomial</td>
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</tr>
<tr>
<td>C</td>
<td>−57.438</td>
<td>Chebyshev equation and coefficients given in ref.</td>
<td></td>
</tr>
</tbody>
</table>

bp/°C: 77.115
Bublik: P/kPa
A: 6.20229
B: 1232.542
C: 216.587

FIGURE 15.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for ethyl acetate.

b.p. = 77.11 °C
15.1.1.7 Propyl acetate

Common Name: Propyl acetate
Synonym: acetic acid propyl ester, propyl ethanoate, n-propyl acetate
Chemical Name: propyl acetate, n-propyl acetate
CAS Registry No: 109-60-4
Molecular Formula: \( \text{C}_5\text{H}_{10}\text{O}_2 \), \( \text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_3 \)
Molecular Weight: 102.132
Melting Point (°C): –93 (Lide 2003)
Boiling Point (°C): 101.54 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
  0.8878 (Weast 1982–83)
  0.8830 (25°C, Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
  115.0 (20°C, calculated-density)
  133.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, \( pK_a \):
  –7.18 (Perrin 1972)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (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 temperature designated * are compiled at the end of this section):

18895 (20°C, shake flask-turbidity, Fühner 1924)
18890 (Fühner 1924; quoted, Hansch et al. 1968)
20380 (estimated, McGowan 1954)
18160 (quoted, Deno & Berkheimer 1960)
18900 (Stephen & Stephen 1963; quoted, Howard 1993)
18895 (shake flask-UV, Hansch et al. 1968)
20430 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
22450 (20°C, literature average, Verschueren 1983)
23000 (Dean 1985)
23000 (20°C, lit. average, Riddick et al. 1986)
22600*, 19800 (20°C, 30°C, shake flask-GC/TC, measured range 0–90.2°C, Stephenson & Stuart 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):

4152* (interpolated-regression of tabulated data, temp range –26.7 to 101.8°C Stull 1947)
\[
\log (P/\text{mmHg}) = [-0.2185 \times 8794.8/(\text{T/K})] + 8.212268; \text{ temp range –38.3 to 89°C (Antoine eq., Weast 1972–73)}
\]
4478 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
\[
\log (P/\text{kPa}) = 6.14362 – 1284.080/(\text{T/K}) – 64.364; \text{ temp range 290.3–398.908 K (Antoine eq., ebulliometry, Ambrose et al. 1981)}
\]
4494 (interpolated-Antoine eq., Boublík et al. 1984)
\[
\log (P/\text{kPa}) = 6.16547 – 1297.186/(210.301 + t/°C); \text{ temp range 17.13–125.8°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)}
\]
\[
\log (P/\text{kPa}) = 6.14152 – 1282.545/(208.628 + t/°C); \text{ temp range 39.8–100.9°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)}
\]
log (P/mmHg) = 7.01615 – 1282.28/(208.6 + t°C), temp range: 39–101°C (Antoine eq., Dean 1985)

(log P/mmHg) = 43.0548 – 3.4692 × 10³/(T/K) – 12.217·log(T/K) + 2.4748 × 10⁻¹⁰·(T/K) + 3.7508 × 10⁻⁶·(T/K)²; temp range 178–549 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):

20.150 (exptl., Hine & Mookerjee 1975)
22.092, 20.62 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
22.09 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C, data presented in graph, ΔH = 43.2 kJ/mol, Kieckbusch & King 1979)
30.50 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
82.91, 203.7, 290.5, 387.3 (40, 60, 70 80°C, equilibrium headspace-GC, Kolb et al. 1992)

ln (1/KAW) = –9.27 + 3971/(T/K), temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)

Octanol/Water Partition Coefficient, log KOW:
1.23 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
1.11 (calculated-activity coeff. γ, Wasik et al. 1981)
1.23 (Hansch & Leo 1985)
1.24 (recommended, Sangster 1989, 1993)
1.24 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KOA:
3.17 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.380, 0.708 (calculated-S, calculated-KOW, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log KOC:
1.288, 2.045 (soil, calculated-S, calculated-KOW, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatileization: based on Henry’s law constant, t½ = 6.5 h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis: 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:

Photolysis half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
Esters 3049

\[ k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 305 \pm 2 \text{ K using relative rate technique for 2-methylpropene (Winer et al. 1977; quoted, Atkinson 1985)} \]

\[ k_{\text{OH}} = (1.7 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (Zetzsch 1982; quoted, Atkinson 1985)} \]

\[ k_{\text{OH}}(\text{calc}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{\text{OH}}(\text{obs.}) = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1985)} \]

\[ k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{\text{OH}}(\text{obs.}) = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR structure-activity relationship, Atkinson 1987)} \]

\[ k_{\text{OH}} = (34.5 \pm 3.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)} \]

\[ k_{\text{OH}} = 3.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \ k(\text{soln}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)} \]

\[ k_{\text{OH}} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)} \]

\[ k_{\text{OH}}(\text{calc}) = 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1996)} \]

Hydrolysis: alkaline hydrolysis rate constant \( k = 0.087 \text{ M}^{-1} \text{ s}^{-1} \text{ at } 25^\circ \text{C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).} \]

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

Half-Lives in the Environment:

Air: photooxidation \( t_\text{v} = 2.4-24 \text{ h} \text{ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);} \]

\[ t_\text{v} = 3.39-6.69 \text{ d, based on exp. rate constant for the vapor-phase reaction with the photochemically produced hydroxyl radical in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993).} \]

### TABLE 15.1.1.7.1

Reported aqueous solubilities of propyl acetate at various temperatures

Stephenson & Stuart 1986

<table>
<thead>
<tr>
<th>t/°C</th>
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<tr>
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<td>9.5</td>
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</tr>
<tr>
<td>80.0</td>
<td>16600</td>
</tr>
<tr>
<td>90.2</td>
<td>13500</td>
</tr>
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</table>
FIGURE 15.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for propyl acetate.

<table>
<thead>
<tr>
<th>Stull 1947</th>
</tr>
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<tbody>
<tr>
<td>summary of literature data</td>
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</tr>
<tr>
<td>–26.7</td>
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<td>64.0</td>
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<tr>
<td>82.0</td>
</tr>
<tr>
<td>101.8</td>
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<tr>
<td>mp/°C</td>
</tr>
</tbody>
</table>
FIGURE 15.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for propyl acetate.
15.1.1.8 Butyl acetate

Common Name: Butyl acetate
Synonym: acetic acid butyl ester, butyl ethanoate, n-butyl acetate, ethanoic acid butyl ester
Chemical Name: butyl acetate, n-butyl acetate
CAS Registry No: 123-86-4
Molecular Formula: C₆H₁₂O₂, CH₃COOCH₂CH₂CH₂CH₃
Molecular Weight: 116.158
Melting Point (°C):
–78 (Lide 2003)
Boiling Point (°C):
126.1 (Lide 2003)
Density (g/cm³ at 20°C):
0.8825 (Weast 1982–83)
0.8764 (Riddick et al. 1986)
Molar Volume (cm³/mol):
132.5 (20°C, calculated-density)
155.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
23.28 (pKₐ, Riddick et al. 1986)
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
43.64, 35.81 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₕus (kJ/mol):
Entropy of Fusion, ∆Sₕus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕus = 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):
23550 (Seidell 1941)
23180 (estimated, McGowan 1954)
4955 (Deno & Berkheimer 1960)
23580 (shake flask-spectrophotometry, Hansch et al. 1968)
7040 (20°C, quoted, Amidon et al. 1975)
6702 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
3936 (Hine & Mookerjee 1975)
5000, 14000 (Verschueren 1983)
4300 (Dean 1985)
8400 (shake flask-radiometric method, Lo et al. 1986)
6800 (20°C, quoted lit. average, Riddick et al. 1986)
6400*, 5200 (19.7°C, 30.3°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson & Stuart 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):
log (P/mmHg) = 8.099 − 1964/(253 + t°C) (Davis 1941)
1560* (24.5°C, measured range 24.5–94.1°C, Usanovich & Dembicij 1959)
9210* (59.74°C, temp range 59.74–126.09°C, Kliment et al. 1964; quoted, Boublík et al. 1984)
1505 (Hoy 1970)
log (P/mmHg) = 6.9688 − 1326.7/(199.2 + t°C); temp range 67.0–130°C (ebulliometry, Sheehan & Langer 1969)
log (P/mmHg) = [–0.2185 × 9300.8/(T/K)] + 8.095046; temp range –21.2 to 118°C (Antoine eq., Weast 1972–73)
1440 (quoted, Hine & Mookerjee 1975)
1333 (20.0°C, Verschueren 1983)
1530, 1138 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 4.7514 – 669.809/(T/°C); temp range 24.5–94.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.25496 – 1432.217/(210.936 + T/°C); temp range 59.74–126°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1529 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 4.7514 – 669.809/(117.657 + T/°C); temp range 60–126°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.13505 – 1355.816/(–70.705 + T/K); temp range 200–579 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
33.44 (exptl., Hine & Mookerjee 1975)
30.50, 31.21 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)
28.51 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 47.6 kJ/mol, Kieckbusch & King 1979)
38.39 (predicted-MCI χ, Nirmalakhandan & Speece 1988)
82.91* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
20.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_AW = 6.400 – 2486/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_OW:
1.73 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
1.69 (calculated-activity coeff. γ, Wasik et al. 1981)
1.82 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
1.78 (24°C, shake flask-GC, Catz & Friend 1989)
1.82 (recommended, Sangster 1989, 1993)
1.78 (recommended, Hansch et al. 1993)

Octanol/Air Partition Coefficient, log K_OA at 25°C:
3.65 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.602, 1.146 (calculated-S, calculated-K_OW, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_OC:
1.531, 2.367 (soil, calculated-S, calculated-K_OW, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, t½:
Volatilization: using Henry’s law constant, t½ ~ 6.1 h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s and an estimated t½ ~ 7.4 d for a 10 m deep similar model river (Lyman et al. 1982; quoted, Howard 1990).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_OH for reaction with OH radical, k_NO3 with NO3 radical and k_O3 with O3 or as indicated, *data at other temperatures see reference: photooxidation t½ = 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
\( k_{\text{OH}}(\text{calc}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \), \( k_{\text{OH}}(\text{obs.}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (SAR structure-activity relationship, Atkinson 1987)

Photooxidation \( t_{\text{v}} = 6.0 \text{ d} \) in air was estimated for the vapor-phase reaction with an average atmospheric OH of \( 8 \times 10^5/\text{cm}^3 \) (GEMS 1986; quoted, Howard 1990)

\( k_{\text{OH}} = (41.5 \pm 3.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

\( k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1989)

Hydrolysis: alkaline hydrolysis rate constant \( k = 0.087 \text{ M}^{-1} \text{ s}^{-1} \) at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

\( t_{\text{v}} = 3.1 \text{ yr} \), 114 d, 11.4 d at pH 7.0, 8.0, 9.0 were estimated, respectively, based on observed acid and base-catalyzed rate constants at 20°C (Mabey & Mill 1978; quoted, Howard 1990).

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

Half-Lives in the Environment:
Air: \( t_{\text{v}} = 2.4–24 \text{ h} \) 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); \( t_{\text{v}} = 6.0 \text{ d} \) was estimated for the vapor-phase reaction with an average atmospheric hydroxyl radical of \( 8 \times 10^5 \text{ per cm}^3 \) (GEMS 1986; quoted, Howard 1990).

**TABLE 15.1.1.8.1**

Reported aqueous solubilities and Henry's law constants of butyl acetate at various temperatures

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<thead>
<tr>
<th>Aqueous solubility</th>
<th>Henry's law constant</th>
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<tr>
<td>Stephenson &amp; Stuart 1986</td>
<td>Kolb et al. 1992</td>
</tr>
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<td><strong>shake flask-GC/TC</strong></td>
<td><strong>equilibrium headspace-GC</strong></td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
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<tr>
<td>0</td>
<td>9600</td>
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<td>7600</td>
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<td>50.0</td>
<td>500</td>
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<tr>
<td>60.2</td>
<td>500</td>
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</tbody>
</table>

**Biodegradation**

**Biotransformation**

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

**Half-Lives in the Environment**

**Air**: \( t_{\text{v}} = 2.4–24 \text{ h} \) 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);

\( t_{\text{v}} = 6.0 \text{ d} \) was estimated for the vapor-phase reaction with an average atmospheric hydroxyl radical of \( 8 \times 10^5 \text{ per cm}^3 \) (GEMS 1986; quoted, Howard 1990).
FIGURE 15.1.1.8.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for butyl acetate.

TABLE 15.1.1.8.2
Reported vapor pressures of butyl acetate at various temperatures and the coefficients for the vapor pressure equations

<table>
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<tr>
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<th>ln $P$ = $A - B/(T/K)$</th>
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<td>(1)</td>
<td>(1a)</td>
</tr>
<tr>
<td></td>
<td>log $P$ = $A - B/(C + t/°C)$</td>
<td>ln $P$ = $A - B/(C + t/°C)$</td>
</tr>
<tr>
<td></td>
<td>(2)</td>
<td>(2a)</td>
</tr>
<tr>
<td></td>
<td>log $P$ = $A - B/(C + T/K)$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>log $P$ = $A - B/(T/K) - C\cdot\log (T/K)$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4)</td>
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</tr>
</tbody>
</table>

Usanovich & Dembicij 1959
in Boublík et al. 1984

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.5</td>
<td>1560</td>
<td>59.74</td>
<td>9210</td>
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<td>33.0</td>
<td>2533</td>
<td>62.35</td>
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Kliment et al. 1964
in Boublík et al. 1984

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Sheehan & Langer 1969
ebulliometry

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FIGURE 15.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for butyl acetate.
15.1.1.9 Pentyl acetate

Common Name: Pentyl acetate
Synonym: acetic acid pentyl ester, amyl acetate, amy lacetic ester, pentyl ethanoate, n-pentyl acetate, ethanoic acid pentyl ester
Chemical Name: \( n \)-amyl acetate, \( n \)-pentyl acetate
CAS Registry No: 628-63-7
Molecular Formula: \( \text{C}_7\text{H}_{14}\text{O}_2 \), \( \text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \)
Molecular Weight: 130.185
Melting Point (°C):
-70.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
149.2 (Lide 2003)
Density (g/cm³ at 20°C):
0.8756 (Weast 1982–83)
0.8766, 0.8719 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
148.5 (20°C, calculated-density)
177.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
24.25 (\( pK_a \), Riddick et al. 1986)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
41.0 (at bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entergy 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. Additional data at other temperatures designated * are compiled at the end of this section):
1730 (shake flask-turbidimeter, McBain & Richards 1946)
1800 (20°C, Verschueren 1983)
1700 (Dean 1985)
1700 (20°C, Riddick et al. 1986)
2200*, 1600 (19.7°C, 30.3°C, shake flask-GC/TC, measured range 0–80°C, Stephenson & Stuart 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\[ \log (P/\text{mmHg}) = 8.078 - 2077/(253 + t/°\text{C}) \] (Davis 1946)
547 (quoted, Hine & Mookerjee 1975)
546 (quoted, Abraham 1984)
1290 (selected lit., Riddick et al. 1986)
\[ \log (P/\text{kPa}) = 5.4315 - 1197/(200 + t/°\text{C}) \]; temp range not specified (Antoine eq., Riddick et al. 1986)
\[ \log (P/\text{kPa}) = 7.356 - 2258.3/(T/\text{K}) \]; temp range 329–423 K (Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{mmHg}) = 7.8848 - 3.0696 \times 10^3/(T/\text{K}) + 2.7085 \log(T/\text{K}) - 1.5165 \times 10^{-2} \times (T/\text{K})^2 \]; temp range 202–598 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
39.29 (exptl., Hine & Mookerjee 1975)
42.10, 42.16 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)
35.94 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, \( \Delta H = 51.4 \text{ kJ/mol} \), Kieckbusch & King 1979)
48.33 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988)
38.39  (calculated-molecular structure, Russell et al. 1992)
24.86  (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log $K_{AW} = 7.167 - \frac{2685}{(T/K)}$ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log $K_{OW}$:
1.70   (calculated, Iwasa et al. 1965)
2.23   (Leo et al. 1969)
2.42   (calculated-V$_j$ and solvatochromic parameters, Leahy 1986)

Octanol/Air Partition Coefficient, log $K_{OA}$:
4.12   (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:
  photooxidation $t_{1/2} = 2.4–24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976).
Hydrolysis:
Biodegradation:
  biodegradation rates $k = 0.054$ d$^{-1}$ with $t_{1/2} = 13$ d in Lester river, $k = 0.069$ d$^{-1}$ with $t_{1/2} = 10$ d in Superior harbor waters and $k = 0.014$ d$^{-1}$ with $t_{1/2} = 50$ d in groundwater (Vaishnav & Babeu 1987).
Biotransformation:
  Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: photooxidation $t_{1/2} = 2.4–24$ h 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).
Surface water: biodegradation $t_{1/2} = 13$ d in Lester river and $t_{1/2} = 10$ d in Superior harbor waters (Vaishnav & Babeu 1987).
Groundwater: biodegradation $t_{1/2} = 50$ d (Vaishnav & Babeu 1987).
Sediment:
Soil:
Biota:

### TABLE 15.1.1.9.1
Reported aqueous solubilities of pentyl acetate at various temperatures

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<td>80.1</td>
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</table>
FIGURE 15.1.1.9.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for pentyl acetate.
15.1.1.10 Methyl acrylate

Common Name: Methyl acrylate
Synonym: acrylic acid methyl ester, methyl 2-propenoate
Chemical Name: methyl acrylate
CAS Registry No: 96-33-3
Molecular Formula: C₄H₆O₂, CH₂=CHCOOCH₃
Molecular Weight: 86.090
Melting Point (°C):
-76.5 (Dean 1985)
Boiling Point (°C):
80.7 (Lide 2003)
Density (g/cm³ at 20°C):
0.9535 (Weast 1982–83; Riddick et al. 1986)
0.9561 (Dean 1985)
Molar Volume (cm³/mol):
90.3 (20°C, calculated-density)
99.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ΔHV (kJ/mol):
29.20, 33.1 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
60000 (Dean 1985)
49400 (Riddick et al. 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
11250 (interpolated-regression of tabulated data, temp range –43.7 to 80.2°C, Stull 1947)
13330 (28.0°C, Stull 1947)
log (P/mmHg) = [–0.2185 × 8598.0/(T/K)] + 8.226778; temp range –43.7 to 80.2°C (Antoine eq., Weast 1972–73)
9330, 14660 (20°C, 30°C, Verschueren 1983)
11000 (Riddick et al. 1986)
3120, 5400, 9090, 11000, 14500, 30000, 70700 (0, 10, 20, 25, 30, 50, 70°C, Riddick et al. 1986)
log (P/kPa) = 6.5561 – 1467.93/(–30.849 + T/K); temp range: 316–354 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 47.0416 – 3.1218 × 10⁴/(T/K) – 14.86 · log(T/K) + 7.1646 × 10⁻³ · (T/K) + 3.4547 × 10⁻⁵ · (T/K)²;
temp range 196–536 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
19.17 (calculated-P/C with selected values)
Octanol/Water Partition Coefficient, log Kow:
0.21 (Tute 1971; Laurence et al. 1972)
0.36 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
0.80 (shake flask-GC, Tanii & Hashimoto 1982)
0.80 (recommended, Sangster 1989)
Octanol/Air Partition Coefficient, log Koa:
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatileization:

Photolysis:

Oxidation: photooxidation t_{1/2} = 2.7–27 h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: first order hydrolysis t_{1/2} = 2.8 yr at pH 7 and 25°C, based on measured base rate constant; acid rate constant k = 1.2 \times 10^{-7} M^{-1} h^{-1} using measured rate constant for ethyl acrylate, resulting a t_{1/2} = 280 yr; base rate constant k = 0.0779 M^{-1} h^{-1} at pH 9 and 25°C with t_{1/2} = 10 d (Roy 1972; quoted, Howard et al. 1991). Biodegradation: aqueous aerobic t_{1/2} = 24–168 h, based on biological screening test data (Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic t_{1/2} = 96–672 h, based on 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} = 2.7–27 h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 to 1–5 d (Kelly et al. 1994).

Surface water: t_{1/2} = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991). Groundwater: t_{1/2} = 48–336 h, based on measured hydrolysis data and estimated 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:
15.1.1.11 Ethyl acrylate

Common Name: Ethyl acrylate
Synonym: acrylic acid ethyl ester, ethyl 2-propenoate, propenoic acid ethyl ester
Chemical Name: ethyl acrylate, \( n \)-ethyl acrylate
CAS Registry No: 140-88-5
Molecular Formula: \( \text{C}_5\text{H}_8\text{O}_2, \text{CH}_2=\text{CHCOOCH}_2\text{CH}_3 \)
Molecular Weight: 100.117
Melting Point (°C):
-71.2 (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
99.4 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
0.9234 (Weast 1982–83; Riddick et al. 1986)
0.9405 (Dean 1985)
Molar Volume (cm\(^3\)/mol):
109.2 (Stephenson & Malanowski 1987)
123.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, \( pK_a \):

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
34.7 (at bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{ fus} = 56 \) J/mol K), \( F \): 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
20000 (Verschueren 1983)
15000 (Dean 1985; 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):
4860* (interpolated-regression of tabulated data, temp range –29.5 to 99.5°C, Stull 1947)
\( \log (P/\text{mmHg}) = [–0.2185 \times 9259.4/(T/K)] + 8.347017 \); temp range –29.5 to 99.5°C (Antoine eq., Weast 1972–73)
3866, 6532 (20°C, 30°C, Verschueren 1983)
5100 (lit average, Riddick et al. 1986)
5140 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
\( \log (P_{\text{vap}}/\text{kPa}) = 7.2103 – 1939.49/(T/K) \); temp range: not specified, (Antoine eq., Riddick et al. 1986)
\( \log (P_0/\text{kPa}) = 6.25041 – 1354.65/(-53.603 + T/K) \); temp range: 244–373 K (Antoine eq., Stephenson & Malanowski 1987)
\( \log (P/\text{mmHg}) = 55.0109 – 3.5904 \times 10^3/(T/K) – 17.694\log(T/K) + 8.051 \times 10^{-3}(T/K) – 4.8864 \times 10^{-13}(T/K)^2 \); temp range 202–553 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m\(^3\)/mol 25°C):
34.041 (calculated-P/C with selected values)
Octanol/Water Partition Coefficient, log \( K_{OW} \):
0.73 (Tute 1971; Laurence et al. 1972)
0.88 (calculated-fragment const. per Rekker 1977, Hermens & Leeuwangh 1982)
0.66 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
1.33 (shake flask-GC, Tani & Hashimoto 1982)
1.32 (recommended, Sangster 1989)
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: photooxidation $t_\text{1/2} = 2.37–22.7$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: overall rate constant $k_\text{H} = 6.3 \times 10^{-6}$ s$^{-1}$ with $t_\text{1/2} = 3.5$ yr at $25^\circ$C and pH 7; acid rate constant $k_\text{A} = 1.2 \times 10^{-13}$ s$^{-1}$ and base rate constant $k_\text{B} = 7.8 \times 10^{-9}$ s$^{-1}$ at $25^\circ$C and pH 7 (Mabey & Mill 1978)

$\text{pH} = 2.8$ yr at pH 7 and $25^\circ$C, based on acid and base catalyzed hydrolysis rate constants; acid rate constant $k_\text{A} = 1.2 \times 10^{-6}$ M$^{-1}$ s$^{-1}$ with $t_\text{1/2} = 244$ yr at pH 5; measured base rate constant $k_\text{B} = 0.078$ M$^{-1}$ h$^{-1}$ with $t_\text{1/2} = 10.4$ d at pH 9 and $25^\circ$C (Howard et al. 1991); calculated rate constant for base-catalyzed hydrolysis $k_\text{B} = 5.0 \times 10^{-2}$ M$^{-1}$ s$^{-1}$ and estimated $t_\text{1/2} \sim 25$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999).

Biodegradation: aqueous aerobic $t_\text{1/2} = 24–168$ h, based on aqueous aerobic screening test data (Price et al. 1974; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_\text{1/2} = 96–672$ 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 $t_\text{1/2} = 2.37–22.7$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: hydrolysis $t_\text{1/2} = 3.5$ yr at $25^\circ$C and pH 7 (Mabey & Mill 1978)

$\text{pH} = 24–168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

Sediment:

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

Biota:

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<th>TABLE 15.1.1.11.1</th>
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FIGURE 15.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl acrylate.
15.1.1.12 Methyl methacrylate

Common Name: Methyl methacrylate
Synonym: methyl 2-methyl-2-propenoate, methyl ester methacrylic acid, methacrylic acid methyl ester, MMA
Chemical Name: 2-methyl-2-propenoic acid methyl ester
CAS Registry No: 80-62-6
Molecular Formula: C₅H₈O₂, H₂C=C(CH₃)COOCH₃
Molecular Weight: 100.117
Melting Point (°C): –47.55 (Lide 2003)
Boiling Point (°C): 100.5 (Lide 2003)
Flash Point (°C): 10
Density (g/cm³ at 20°C): 0.9440 (Weast 1982–83)
Molar Volume (cm³/mol): 106.6 (25°C, Stephenson & Malanowski 1987)
121.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
40.7, 36.0 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion ∆Hₜ (kJ/mol):
Entropy of Fusion, ∆Sₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₜ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
16000 (Dean 1985)
15000 (USEPA 1985; ENVIROFATE; ISHOW)
15900 (Yalkowsky et al. 1987)
15600 (20°C, 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):
5332*, 4888 (25.5°C, interpolated-regression of tabulated data, temp range –30.5 to 101°C, Stull 1947)
1315* (3.44°C, temp range –45.26 to 3.44°C, Bywater 1952; quoted, Boublík et al. 1984)
log (P/mmHg) = [–0.2185 × 8794.9/(T/K)] + 8.140942; temp range –30.5 to 101°C (Antoine eq., Weast 1972–73)
3732, 5333 (20°C, 26°C, Verschueren 1977, 1983)
7003* (32.49°C, temp range 32.49–99.855°C, Boublík & Aim 1979; quoted, Boublík et al. 1984)
5333 (25.5°C, Weast 1982–83)
4440 (extrapolated average-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 3.20496 – 4017.882/(126.685 + t°C); temp range –45.26 to 3.44°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
log (P/kPa) = 6.19400 – 1315.670/(213.490 + t°C); temp range: 32.41–99.855°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
4846 (extrapolated-Antoine equation, Dean 1985)
log (P/mmHg) = 8.4092 – 2050.5/(274.4 + t°C); temp range: 39–89°C (Antoine eq., Dean 1985, 1992)
5100 (lit. average, Riddick et al. 1986)
log (P/kPa) = 7.83859 – 2126.21/(T/K); temp range 0–30°C (Antoine eq., Riddick et al. 1986)
5081, 5020 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
log (Pₗ/kPa) = 6.63751 – 1597.9/(–28.76 + T/K); temp range: 293–374 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \( \left( \frac{P}{kP} \right) = 6.43088 - 1461.197/(–43.15 + T/K) \); temp range: 293–373 K (Antoine eq., II, Stephenson & Malanowski 1987)

\[
\log (P/mmHg) = 106.896 - 5.2741 \times 10^3/(T/K) - 37.654\log(T/K) + 1.862 \times 10^2\times(T/K) - 3.6507 \times 10^13\times(T/K) \;
\]
temp range 225–564 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 24.31 (calculated-P/C, USEPA 1985)
- 32.823 (calculated-P/C, Howard 1989)
- 32.09 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log \( K_{ow} \):
- 0.73 (Tute 1971; Laurence et al. 1972)
- 0.70 (shake flask, Fujisawa & Masuhara 1981)
- 0.67 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
- 1.36 (CLOGP, Hansch & Leo 1982)
- 1.38 (shake flask-GC, Tani & Hashimoto 1982)
- 0.79 (calculated-f const. as per Lyman et al. 1982, USEPA 1985)
- 1.38 (recommended, Sangster 1989)
- 1.38 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log \( BCF \):
- –0.03 (correlated as per Veith et al. 1979 for aquatic organisms, USEPA 1985)
- 0.55 (calculated-\( K_{ow} \), Howard 1989)

Sorption Partition Coefficient, log \( K_{oc} \):
- 1.80 (calculated-\( K_{ow} \) as per Lyman et al. 1982, USEPA 1985)
- 1.94 (calculated-\( K_{ow} \), Howard 1989)
- 0.74 (calculated-\( K_{ow} \), Kollig 1993)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\text{1/2} \):
- Volatilization: \( t_\text{1/2} = 6.3 \text{ h} \) from model river water (Lyman et al. 1982; quoted, Howard 1989).
- Photolysis: photodegradation \( t_\text{1/2} = 2.7 \text{ h} \) in air of urban areas and \( t_\text{1/2} > 3 \text{ h} \) in rural areas (Joshi et al. 1982; quoted, Howard 1989) (CHEMFATE; Hazardous Substance Databank).
- Oxidation: photooxidation \( t_\text{1/2} = 1.1–9.7 \text{ h} \) in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
- Hydrolysis: alkaline hydrolysis rate constant at 25°C, \( k = 171 \text{ M}^{-1}\text{ h}^{-1} \) (Sharma & Sharma 1970; quoted, Ellington et al. 1987; Ellington 1989);
  - alkaline catalyzed rate constant \( k(\text{exptl}) = 200 \text{ M}^{-1}\text{ h}^{-1} \) at 25°C with estimated \( t_\text{1/2} = 3.9 \text{ yr} \) at pH 7 and \( t_\text{1/2} = 14 \text{ d} \) at pH 9 (Ellington et al. 1987; quoted, Ellington 1989; Howard 1989; Howard et al. 1991; Kollig 1993);
  - hydrolysis \( t_\text{1/2} = 4 \text{ yr} \) at pH 7 and 25°C; base rate constant \( k = 200 \text{ M}^{-1}\text{ h}^{-1} \) with \( t_\text{1/2} = 14.4 \text{ d} \) at pH 9 based on measured rate constant at 25°C and pH 11 (Howard et al. 1991)
  - \( k(\text{calc}) = 9.0 \times 10^{-3} \text{ M}^{-1}\text{ s}^{-1} \), \( 2.6 \times 10^{-2} \text{ M}^{-1}\text{ s}^{-1} \) for neutral and base-catalyzed hydrolysis and estimated \( t_\text{1/2} = 8 \text{ d} \) in aqueous solutions at pH 8.8 (Freidig et al. 1999)
- Biodegradation: completely degraded by activated sludge in approximately 20 h (Slave et al. 1974; quoted, EPA 1985; Howard 1989; Hazardous Substance Databank);
  - expert systems survey found that both aerobic ultimate degradation in receiving waters and anaerobic ultimate degradation were within a month and aerobic primary degradation in receiving waters was within few days (Boethling et al. 1989);
  - aqueous aerobic \( t_\text{1/2} = 168–672 \text{ h} \), based on unacclimated screening test data (Pahren & Bloodgood 1961; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic \( t_\text{1/2} = 672–2688 \text{ h} \), based on unacclimated 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_½ = 1.1–9.7 h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 to 1–5 d (Kelly et al. 1994).
Surface water: t_½ = 168–672 h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).
Groundwater: t_½ = 336–1344 h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: t_½ = 168–672 h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).
Biota:

**TABLE 15.1.12.1**
Reported vapor pressures of methyl methacrylate at various temperatures and the coefficients for the vapor pressure equations

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<th>Stull 1947</th>
<th>Bywater 1952</th>
<th>Boublik &amp; Aim 1979</th>
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<tr>
<td>summary of literature data</td>
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<td>in Boublik et al. 1984</td>
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</table>
**FIGURE 15.1.12.1** Logarithm of vapor pressure versus reciprocal temperature for methyl methacrylate.
15.1.2 AROMATIC ESTERS

15.1.2.1 Methyl benzoate

Common Name: Methyl benzoate
Synonym: benzoic acid methyl ester
Chemical Name: methyl benzoate
CAS Registry No: 93-58-3
Molecular Formula: C₈H₆O₂, C₆H₅COOCH₃
Molecular Weight: 136.149
Melting Point (°C):
  -12.4  (Lide 2003)
Boiling Point (°C):
  199  (Lide 2003)
Density (g/cm³ at 20°C):
  1.08854, 1.08377  (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
  125.0  (Stephenson & Malanowski 1987)
  151.2  (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
  41.18, 55.84  (normal bp, 25°C, Dreisbach 1955)
  43.18, 55.568  (normal bp, 25°C, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hₕₑₚ (kJ/mol):
  9.736  (Dreisbach 1955; Riddick et al. 1986)
Entropy of Fusion, ∆Sₕₑₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sₕₑₚ = 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):
  1524  (titration, Booth & Everson 1948)
  4018  (Hine & Mookerjee 1975)
  2100  (20°C, quoted, Riddick et al. 1986)
  1600  (calculated-MCI χ, Nirmalakhandan & Speece 1988)
  2130*, 2820 (20.1°C, 29.6°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson & Stuart 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  log (P/mmHg) = 7.48253 – 1974.6/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
  52.58  (calculated by formula, Dreisbach 1955)
  log (P/mmHg) = 7.07832 – 1656.25/(195.23 + t/°C); temp range: 100–260°C (Antoine eq. for liquid state, Dreisbach 1955)
  log (P/mmHg) = [–0.2185 × 12077.2/(T/K)] + 8.509910; temp range: 39–199.5°C (Antoine eq., Weast 1972–73)
  77.6  (extrapolated-Antoine eq., Dean 1985)
  log (P/mmHg) = 6.60743 – 1974.6/(230.0 + t/°C); temp range 111–199°C (Antoine eq., Dean 1985, 1992)
  52.58  (quoted lit. average, Riddick et al. 1986)
  log (P/kPa) = 6.60743 – 1974.6/(230 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
  54.5  (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P₉/kPa) = 8.183 – 2816.6/(T/K); temp range 283–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log \((P_{\text{L/kPa}}) = 6.20322 - 1656.25/(−77.92 + T/\text{K})\); temp range: 383–533 K (Antoine eq.-II, Stephenson & Malanowski 1987)

\[
\log (P_{\text{mmHg}}) = −13.6342 −2.9133 \times 10^3/(T/\text{K}) + 11.773 \log (T/\text{K}) −2.3979 \times 10^{−2}(T/\text{K})^2;
\]

temp range 261–693 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 1.80 (calculated-\(C_m/C_a\), Hine & Mookerjee 1975)
- 2.48 (calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
- 2.15 (HPLC-RT correlation, D’Amboise & Hanai 1982)
- 2.22 (HPLC-k’ correlation, Haky & Young 1984)
- 2.10 (recommended, Klein et al. 1988)
- 2.15 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 2.20 (recommended, Sangster 1989)
- 2.12 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log \(BCF\):

Sorption Partition Coefficient, log \(K_{\text{OC}}\):
- 2.30, 2.01, 1.98 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.89 (calculated-MCI \(\chi\), Meylan et al. 1992)
- 2.10 (quoted or calculated-QSAR MCI \(\chi\), Sabljic et al. 1995)
- 2.14; 2.57, 2.14, 1.94, 2.16, 1.89 (soil: calculated-\(K_{\text{OW}}\); 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:

Photolysis:

Oxidation:

Hydrolysis: overall rate constant \(k_h = 1.90 \times 10^{-10} \text{s}^{-1}\) with \(t_{1/2} = 118 \text{yr at 25°C and pH 7}\) (Mabey & Mill 1978)

alcaline hydrolysis rate constant \(k = 0.0794 \text{M}^{-1} \text{s}^{-1}\) (Drossman et al. 1988, quoted, Collette 1990)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:
Surface water: hydrolysis \(t_{1/2} = 118 \text{yr at 25°C and pH 7}\) (Mabey & Mill 1978)

Groundwater:

Sediment:

Soil:

Biota:
TABLE 15.1.2.1.1
Reported aqueous solubilities of methyl benzoate at various temperatures
Stephenson & Stuart 1986

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<th>t/°C</th>
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</table>

FIGURE 15.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for methyl benzoate.
15.1.2.2 Ethyl benzoate

Common Name: Ethyl benzoate
Synonym: benzoic acid ethyl ester, ethyl benzenecarboxylate
Chemical Name: benzoic acid ethyl ester, ethyl benzenecarboxylate, ethyl benzoate
CAS Registry No: 93-89-0
Molecular Formula: C₉H₁₀O₂, C₆H₅COOC₂H₅
Molecular Weight: 150.174
Melting Point (°C):
  –34 (Lide 2003)
Boiling Point (°C):
  212 (Lide 2003)
Density (g/cm³ at 20°C):
  1.0468 (Weast 1982–83)
  1.0511, 1.0372 (15°C, 30°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
  175.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
  40.5 (Riddick et al. 1986)
Enthalpy of Fusion, ΔHₘₕ (kJ/mol):
Entropy of Fusion, ΔSₘₕ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₘₕ = 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):
  720 (Seidell 1941; quoted, Andrews & Keefer 1950)
  598 (Deno & Berkheimer 1960)
  702 (calculated-Kᵢₒₑₑ, Hansch et al. 1968)
  510 (calculated-Kᵢₒₑₑ, Yalkowsky & Morozowich 1980)
  2026 (calculated-Kᵢₒₑₑ and mp, Amidon & Williams 1982),
  807 (calculated-intrinsic molar volume V₁ and solvatochromic parameters, Leahy 1986)
  1090 (calculated-intrinsic molar volume V₁ and solvatochromic parameters, Kamlet et al. 1987)
  464 (calculated-intrinsic molar volume V₁ and mp, Kamlet et al. 1987)
  500 (20°C, Riddick et al. 1986)
  926 (calculated-fragment const., Wakita et al. 1986)
  398 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
  850*, 810 (19.6°C, 30. °C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson & Stuart 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  42.1 (extrapolated-regression of tabulated data, temp range 44–213.4°C, Stull 1947)
  log (P/mmHg) = [–0.2185 x 11981.5/(T/K)] + 8.279591; temp range 44–213.4°C (Antoine eq., Weast 1972–73)
  24.0 (20°C, quoted lit., Riddick et al. 1986)
  log (P/kPa) = 7.7579 – 2750.0/(T/K); temp range 90–140°C (Antoine eq., Riddick et al. 1986)
  log (P/kPa) = 7.1599 – 2500.0/(T/K); temp range 140–220°C (Antoine eq., Riddick et al. 1986)
  27.5 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
  log (P/kPa) = 6.81152 – 2174.3/(-34.071 + T/K); temp range 358–487 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/kPa) = 8.23958 – 2922.167/(T/K); temp range 288–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)
Esters

log (P/mmHg) = 40.8047 − 3.9985 × 10^{3}/(T/K) − 11.793·log (T/K) + 4.0697 × 10^{-3}·(T/K) − 1.2372 × 10^{-13}·(T/K)^2;
temp range 238–698 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
10.298 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW}:
2.62 (calculated, Hansch et al. 1968)
2.20 (shake flask-spectrophotometry, Yaguzhinskii et al. 1973)
2.64 (Valvani et al. 1981, Amidon & Williams 1982)
2.64 (shake flask-HPLC, Nielsen & Bundgaard 1988)
2.60 (recommended, Klein et al. 1988)
2.64 (recommended, Sangster 1989)
2.66, 2.89, 2.90 (centrifugal partition chromatography CPC-RV, Gluck & Martin 1990)
2.70 ± 0.15, 2.63 ± 0.57 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k' correlation, Cichna et al. 1995)
2.64 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.25, 2.17, 2.43 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
2.16 (calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.30 (quoted or calculated-QSAR MCI 1χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: overall rate constant k_h = 3.0 × 10^{-9} s^{-1} with t_{½} = 7.3 yr at 25°C and pH 7 (Mabey & Mill 1978)
alkaline hydrolysis rate constant k = 0.0316 M^{-1} s^{-1} (Drossman et al. 1988, quoted, Collette 1990)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: hydrolysis t_{½} = 7.3 yr at 25°C and pH 7 (Mabey & Mill 1978)
Groundwater:
Sediment:
Soil:
Biota:
TABLE 15.1.2.2.1
Reported aqueous solubilities of ethyl benzoate at various temperatures
Stephenson & Stuart 1986

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</table>

FIGURE 15.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl benzoate.
15.1.2.3 *n*-Propyl benzoate

Common Name: *n*-Propyl benzoate
Synonym: benzoic acid *n*-propyl ester, propyl benzenecarboxylate
Chemical Name: benzoic acid *n*-propyl ester, propyl benzenecarboxylate, propyl benzoate
CAS Registry No: 2315-68-6
Molecular Formula: C_{10}H_{12}O_{2}, C_{6}H_{5}COOCH_{2}CH_{2}CH_{3}
Molecular Weight: 164.201

Melting Point (°C): ~51.6 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C): 211 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C): 1.0232 (Riddick et al. 1986)
Molar Volume (cm³/mol):
- 160.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
- 199.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ΔHV (kJ/mol):
- 51.92; 49.75 (25°C; bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 350 (quoted exptl., Kamlet et al. 1987)
- 292 (calculated-intrinsic molar volume V₁ and solvatochromic parameters, Kamlet et al. 1987)
- 140 (calculated-intrinsic molar volume V₁ and mp, Kamlet et al. 1987)
- 966 (calculated-MCI χ, Nirmalakhandan & Speece 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 133.3 (54.6°C, summary of literature data, temp range 54.6–231°C, Stull 1947)
- log (P/mmHg) = [–0.2185 × 12318.7/(T/K)] + 8.237827; temp range 54.6–231°C (Antoine eq., Weast 1972–73)
- log (P/kPa) = 7.42756 – 2172.71/(T/K); temp range 80–160°C (Antoine eq., Riddick et al. 1986)
- log (P₁/kPa) = 6.68614 – 2165.28/(–41.593 + T/K); temp range 327–504 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
- 1.80 (shake flask-HPLC, Nielsen & Bundgaard 1988)
- 3.18 (recommended, Sangster 1989)
- 3.01 (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, $t_{1/2}$:

Half-Lives in the Environment:
15.1.2.4 Benzyl benzoate

Common Name: Benzyl benzoate
Synonym: benzoic acid benzyl ester, phenylmethyl benzoate, benzyl benzenecarboxylate, benzyl phenylformate, benzenoate
Chemical Name: benzyl benzoate, phenylmethyl benzoate, benzyl benzenecarboxylate
CAS Registry No: 120-51-4
Molecular Formula: C_{14}H_{12}O_{2}, C_6H_5COOCH_2C_6H_5
Molecular Weight: 212.244
Melting Point (°C): 19.4 (Riddick et al. 1986)
Boiling Point (°C): 323.5 (Lide 2003)
Density (g/cm³ at 20°C): 1.1121 (25°C, Weast 1982–83)
Molar Volume (cm³/mol): 243.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pKₐ:
Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):
53.56 (at normal bp, Hon et al. 1976)
77.8; 53.6 (25°C bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hᵤₛ (kJ/mol):
Entropy of Fusion, ∆Sᵤₛ (J/mol K):
Fugacity Ratio at 25°C (assuming ∆Sᵤₛ = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
15.73 (Seidell 1941; quoted, Deno & Berkheimer 1960)
61.21 (calculated-intrinsic molar volume Vᵢ and solvatochromic parameters, Leahy 1986)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/mmHg) = -1.654 – 4.6284 × 10⁻³/(T/K) + 7.363-log (T/K) – 1.8259 × 10⁻²-(T/K) + 7.4580 × 10⁻⁶-(T/K)²;
temp range 293–820 K (vapor pressure eq., Yaws et al. 1994)
0.0178, 0.0107, 0.0135, 0.295, 0.0603 (GC-RT correlation, Sugden’s parachor method, McGowan’s parachor method, calculated-MCI, calculated-MW, Tsuzuki 2001)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.57 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 3.86 (quoted, calculated-$V_I$ and solvatochromic parameters, Taft et al. 1985)
- 4.00 (quoted, calculated-$V_I$ and solvatochromic parameters, Leahy 1986)
- 3.97 (recommended value, Sangster 1989)

Bioconcentration Factor, log BCF:

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

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:
  - Hydrolysis: overall rate constant $k_h = 8.0 \times 10^{-10}$ s⁻¹ with $t_{1/2} = 27$ yr at 25°C and pH 7 (Mabey & Mill 1978)
  - Alkaline hydrolysis rate constant $k = 0.00794$ M⁻¹ s⁻¹ (Mabey et al. 1978; quoted, Collette 1990)
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air:
- Surface water: hydrolysis $t_{1/2} = 27$ yr at 25°C and pH 7 (Mabey & Mill 1978)
- Groundwater:
- Sediment:
- Soil:
- Biota:
15.1.3 Phthalate esters

15.1.3.1 Dimethyl phthalate (DMP)

Common Name: Dimethyl phthalate
Synonym: DMP, 1,2-benzenedicarboxylic acid dimethyl ester, dimethyl-1,2-benzenedicarboxylate, methyl Common phthalate, α-dimethylphthalate, phthalic acid dimethyl ester
Chemical Name: dimethyl phthalate, dimethyl-α-phthalate, methyl phthalate
CAS Registry No: 131-11-3
Molecular Formula: C_{10}H_{10}O_{4}, α-C_{6}H_{4}(COOCH_{3})_{2}
Molecular Weight: 194.184
Melting Point (°C):
5.5 (Lide 2003)
Boiling Point (°C):
283.7 (Lide 2003)
Density (g/cm³ at 20°C):
1.189 (25°C, Fishbein & Albro 1972)
1.1905 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
162.8 (calculated-density, Stephenson & Malanowski 1987)
206.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
78.66 (Small et al. 1948)
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: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):
3965 (Deno & Berkheimer 1960)
5000 (20°C, Fishbein & Albro 1972)
4000 (32°C, from Monsanto Chemical Co. data sheets, Peakall 1975)
4320 ± 37 (shake flask-GC, Wolfe et al. 1980b; Wolfe et al. 1980a)
4290 (20°C, shake flask-UV, Leyder & Boulanger 1983)
3900 ± 20 (0°C, Verschueren 1983)
4000 ± 60 (shake flask-HPLC/UV, Howard et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
40* (82°C, ebulliometry, measured range 82–151°C, Gardner & Brewer 1937)
log (P/mmHg) = 9.117 –1496.375/(T/K); temp range 82–151°C (Antoine eq. derived by Kim 1985 from exptl data of Gardner & Brewer 1937)
0.863* (extrapolated-regression of tabulated data, temp range 100.3–288.7°C Stull 1947)
0.245 (effusion method, extrapolated-Antoine eq., Small et al. 1948)
log (P/mmHg) = 11.06 – 4113/(T/K); temp range 32–55°C or pressure range 5 × 10⁻² to 10⁻⁴ mmHg (Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)
0.559 (20°C, calculated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 14922.2/(T/K)] + 8.747053; temp range 100.3–287°C (Antoine eq., Weast 1972–73)
0.445 (gas saturation, extrapolated, measured range 60–100°C, Potin-Gautier et al. 1982)
log (P/mmHg) = 8.899 – 3332.764/(T/K); temp range 60–100°C (Antoine eq., Potin-Gautier et al. 1982)

log (P/kPa) = 3.64598 – 699.876/(51.372 + t°C); temp range 82–151°C (Antoine eq. from reported expetl. data, Boublik et al. 1984)

log (P/mmHg) = 4.52232 – 700.31/(51.42 + t/°C); temp range 82–151°C (Antoine eq., Dean 1985, 1992)

0.220 (gas saturation-HPLC/UV, Howard et al. 1985; quoted, Howard et al. 1986; Howard 1989; Banerjee et al. 1990)

0.245, 0.863 (extrapolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)

log (P/kPa) = 10.185 – 4113/(T/K); temp range 304–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 8.095 – 3327/(T/K); temp range 371–547 K (Antoine eq.-II, Stephenson & Malanowski 1987)

1.190 (GC-RT correlation, Hinckley et al. 1990)

log (P/mmHg) = 12.6974 – 4.1989 × 10³/(T/K) + 0.3463·log(T/K) – 7.6524 × 10⁻³·(T/K) + 3.349 × 10⁻⁶·(T/K)²; temp range 272–766 K (vapor pressure eq., Yaws et al. 1994)

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

0.111 (calculated-P/C, Fishbein & Albro 1972)

0.111 (calculated-P/C, Wolfe et al. 1980a)

0.011 (calculated as per Lyman et al. 1982; quoted, Howard 1989)

0.218 (20°C, calculated-P/C, Mabey et al. 1982)

0.012 (selected, Staples et al. 1997)

0.00978 (calculated-QSPR, Cousins & Mackay 2000)

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

1.61 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1983)

1.56 (HPLC-RT correlation, Veith et al. 1980)

1.62, 1.82 (HPLC-‘K’ correlations, McDuffie 1981)

1.53 (20°C, shake flask-UV, Leyder & Boulanger 1983)

1.47, 1.90 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)

1.56 (shake flask, unpublished data, Hansch & Leo 1985; 1987)

1.66 (shake flask, average from interlaboratory study, Renberg et al. 1985)

1.74, 1.61 (HPLC, RP-TLC, average from interlaboratory study, Renberg et al. 1985)

1.62 (HPLC-RT correlation, Eadsforth 1986)

1.46 (shake flask-HPLC/UV, Nielsen & Bundgaard 1989)

1.56 (recommended, Sangster 1993)

1.56 (recommended, Hansch et al. 1995)

1.61 (recommended, Staples et al. 1997)

1.54 (micro-emulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

7.01 (calculated-QSPR, Cousin & Mackay 2000)

Bioconcentration Factor, log BCF:

0.67 (calculated-K_{OW}, Veith et al. 1979, 1980)

1.76 (bluegill sunfish, Barrows et al. 1980)

1.76 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1983)

1.42 (bacteria, calculated-K_{OW} Wolfe et al. 1980a)

0.49–0.8, 0.67–0.78 (shrimp, fish, Wofford et al. 1981)

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

0.77 (sheepshead minnow, quoted from Wofford et al. 1981, Zaroogian et al. 1985)

1.76, 2.22 (quoted, calculated-MCI $\chi$, Sabljic 1987)

0.67, 0.73 (brown shrimp, sheepshead minnow, quoted, Howard 1989)

1.76 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

1.64 (soil, estimated, Kenaga 1980)

2.20 (soil, estimated-K_{OW}, Wolfe et al. 1980a)
1.74 (soil/sediment, Osipoff et al. 1981)
1.24 (sediment-water, calculated-\(K_{OW}\), Mabey et al. 1982)
1.52 (sediment, calculated-\(K_{OW}\), Pavlou & Weston 1983, 1984)
2.69 (activated carbon, calculated- MC\(1\), Blum et al. 1994)
1.20 (calculated-\(K_{OW}\), Kollig 1993)
1.60 (quoted or calculated-QSAR MC\(1\), Sabljic et al. 1995)
4.70 (suspended solids, calculated-\(K_{d}\) assuming a 0.10 organic carbon fraction, Staples et al. 1997)
1.64, 2.14; 2.16, 1.87, 2.53, 1.83, 1.67 (soil: quoted lit., calculated-\(K_{OW}\); HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization: estimated \(t_{1/2} = 46\) d from a river of 1 m deep with 1.0 m/s current and a 3.0 m/s wind using calculated Henry’s law constant and considering the volatilization rate being controlled by the diffusion through the air layer (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: direct \(k_{P} = 2 \times 10^{-4}\) h\(^{-1}\) (EXAMS model, Wolfe et al. 1980a);

abiotic degradation \(t_{1/2} = 3500\) h for direct sunlight in surface waters and \(t_{1/2} = 12.7\) h in pure water but reduced to 2.8 h in the presence of \(NO_2\) when irradiated with a UV lamp through a Pyrex filter (Howard 1989)

Indirect photolysis rate \(k = 0.048\) d\(^{-1}\) with \(t_{1/2} = 14.4\) d in air (Peterson & Staples 2003)

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

\(k_{aq.} = 18\) M\(^{-1}\) s\(^{-1}\) for reaction with free radical in aqueous environment (Wolfe et al. 1980a)

\(k_{aq.} = 23.8\) h (estimated, Howard 1989)

Hydrolysis: \(k_{acidi-catalyzed} = 0.04\) M\(^{-1}\) h\(^{-1}\), \(k_{alkaline} = 2.5 \times 10^2\) M\(^{-1}\) h\(^{-1}\); phthalates are susceptible to alkaline hydrolysis, with theoretical \(t_{1/2} = 1.0\) yr to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

\(k_{second-order alkaline} = 6.9 \times 10^{-2}\) M\(^{-1}\) s\(^{-1}\) at pH 8 and 30°C, and \(t_{1/2} = 4\) months for hydrolytic degradation in the eutrophic lake system (Wolfe et al. 1980b; quoted, Kollig 1993)

\(k_{second-order alkaline} = 6.9 \times 10^{-2}\) M\(^{-1}\) s\(^{-1}\) at pH 10–12 and 30°C in water with \(t_{1/2(calc)} = 3.2\) yr at pH 7 (Callahan et al. 1979)

hydrolysis half-lives: \(t_{1/2} = 3.2\) yr under natural conditions at 30°C, \(t_{1/2} = 11.6\) d at 30°C and \(t_{1/2} = 25\) d at 18°C

Hydrolysis half-lives: \(t_{1/2} = 3.2\) yr under natural conditions at 30°C, \(t_{1/2} = 11.6\) d at 30°C and \(t_{1/2} = 25\) d at 18°C

Biodegradation: calculated rate constant \(k = (9.49 \pm 0.41) \times 10^2\) min\(^{-1}\) from retention times in reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O’Grady et al. 1985); significant degradation with rapid adaption within 7 d in an aerobic environment with a rate \(k > 0.5\) d\(^{-1}\) (Tabak et al. 1981; quoted, Mills et al. 1982); biodegradation rate constant \(k = 1.2 \times 10^{-2}\) mL-cell\(^{-1}\)d\(^{-1}\) in river die-away test (Scow 1982); 58–88% mineralization in 7 d in municipal digested sludge (Horowitz et al. 1982); rate constant \(k = 0.364\) d\(^{-1}\) which corresponds to \(t_{1/2} = 1.90\) d in shake flask biodegradation experiments (Sugatt et al. 1984);

greater than 90% of DMP was degraded within 40 d in digested sludge (Shelton et al. 1984); biodegraded in excess of 90% in activated sludge systems in less than 24 h (O’Grady et al. 1985); soil-water biodegradation studies showed that 85% loss in Brookem County soil after 120 hours and 75% loss in leachate sprayed soil after 48 h (Russell et al. 1985);
anaerobic digestion of sludge with a first-order $k = 8.9 \times 10^{-3}$ h$^{-1}$ and $t_{1/2} = 78$ h (Ziogou et al. 1989); aqueous aerobic $t_{1/2} = 24–168$ h, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data; aqueous anaerobic $t_{1/2} = 96–672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$ (aerobic) = 3 d, $t_{1/2}$ (anaerobic) = 28 d in natural waters (Capel & Larson 1995)

$k = 0.0290$ h$^{-1}$ with $t_{1/2} = 23.9$ h for microbial degradation by anaerobic sludge (Wang et al. 2000)

Aerobic biodegradation in aquatic environments, first order $k = 0.5$ d$^{-1}$ with $t_{1/2} = 1.39$ d in river water, $k = 0.5$ d$^{-1}$ with $t_{1/2} = 1.39$ d in MITI inoculum (Peterson & Staples 2003)

Aerobic biodegradation in soil, pseudo-first-order rate $k = 0.36$ d$^{-1}$ with $t_{1/2} = 1.93$ d in agitated aqueous suspension, and $k = 0.40$ d$^{-1}$ with $t_{1/2} = 1.70$ d at 30°C in garden soil. For anaerobic degradation, first order rate $k = 0.25–0.696$ d$^{-1}$ with $t_{1/2} = 2.8–1.0$ d in digester sludge, batch incubation; $k = 0.033$ d$^{-1}$ with $t_{1/2} = 21$ d in flood soil (Peterson & Staples 2003)

Biodegradation: estimated rate constant $k \approx 5.2 \times 10^{-6}$ mL cell$^{-1}$ h$^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982).

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

$\text{depuration} t_{1/2} = 24–48$ h from bluegill sunfish (Barrows et al. 1980).

$k_2 = 27.7$ d$^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 2.37$ d$^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 23.8$ h for reaction with hydroxyl radicals (Howard 1989);

$\text{t}_{1/2} = 112–1118$ 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 to 5 d (Kelly et al. 1994).

$\text{t}_{1/2} = 14.41$ d based on photooxidation reaction rate with OH radical, indirect photolysis $t_{1/2} = 14.4$ d (Peterson & Staples 2003)

Surface water: estimated $t_{1/2} < 0.3$ d in river waters (Zoeteman et al. 1980);

mineralization $t_{1/2} \sim 7$ d in municipal digested sludge (Horowitz et al. 1982);

biodegradation $t_{1/2} = 1.90$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984);

$\text{t}_{1/2} < 192–264$ h by biodegradation in fresh river water, $t_{1/2} = 12$ h in Rhine River, an estimated $t_{1/2} \sim 13–27$ h in a modelling study of simulated ecosystem; abiotic degradation $t_{1/2} = 12.7$ h in pure water and $t_{1/2} = 2.8$ h in the presence of nitrogen dioxide when irradiated with a UV lamp (Howard 1989);

overall degradation $t_{1/2} = 24–168$ h, based on unacclimated river die-away test data (Howard et al. 1991)

Biodegradation $t_{1/2}$ (aerobic) = 1 d, $t_{1/2}$ (anaerobic) = 4 d in natural waters (Capel & Larson 1995)

$k_{\text{exptl}} = (0.20 \pm 0.10)$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 21- 1°C, with $t_{1/2} = 1.9$ d at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}$ (aerobic) = 1 d, $t_{1/2}$ (anaerobic) = 4 d and $t_{1/2} = 1200$ at pH 7, $t_{1/2} = 0.026$ d at pH 12 in natural waters (Capel & Larson 1995)

$\text{t}_{1/2} = 0.5–1.39$ d for biodegradation in aerobic aquatic environments (Peterson & Staples 2003)

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

Sediment:

Soil: biodegradation $t_{1/2} < 5$ d (aerobic) and $t_{1/2} \sim 20$ d (anaerobic) in a garden soil (Shanker et al. 1985);

$\text{t}_{1/2} = 10–50$ d, via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$\text{t}_{1/2} = 24–168$ h, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data (Howard et al. 1991)

Biodegradation in aerobic soil: $t_{1/2} = 1.93$ d in agitated aqueous suspension and $t_{1/2} = 1.70$ d in garden soil (Peterson & Staples 2003)

Biota: $24 < t_{1/2} < 48$ h depuration half-life in tissues of bluegill sunfish in 21 d-exposure experiment (Barrows et al. 1980; quoted, Howard 1989);

$\text{t}_{1/2} = 23.9$ h for microbial degradation by anaerobic sludge (Wang et al.2000).
**TABLE 15.1.3.1.1**

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

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

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**FIGURE 15.1.3.1.1** Logarithm of vapor pressure versus reciprocal temperature for dimethyl phthalate.
15.1.3.2 Diethyl phthalate (DEP)

Common Name: Diethyl phthalate
Synonym: DEP, ethyl phthalate
Chemical Name: phthalic acid diethyl ester, ethyl phthalate, 1,2-benzenedicarboxylic acid ethyl ester
CAS Registry No: 84-66-2
Molecular Formula: C₁₂H₁₄O₄, C₆H₄(COOC₂H₅)₂
Molecular Weight: 222.237
Melting Point (°C):
  −40.5 (Patty 1963; Fishbein & Albro 1972; Lide 2003)
Boiling Point (°C):
  295 (Lide 2003)
Density (g/cm³ at 20°C):
  1.1175 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
  198.9 (20°C, calculated-density, Stephenson & Malanowski 1987)
  254.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  82.42 (Small et al. 1948)
Enthalpy of Fusion, ΔHₐ (kJ/mol):
Entropy of Fusion, ΔSₐ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₐ = 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):
  598 (Deno & Berkheimer 1960)
  1000 (20°C, Fishbein & Albro 1972)
  1000 (32°C, from Monsanto Chemical Co., data sheets, Peakall 1975)
  896 (shake flask-GC, Wolfé et al. 1980b)
  1200* (20°C, elution chromatography, UV, Schwarz & Miller 1980)
  7028 (shake flask-LSC, Veith et al. 1980)
  928 (20°C, shake flask-UV, Leyder & Boulanger 1983)
  1080 (shake flask-HPLC/UV, Howard et al. 1985)
  680 (measured, Russell & McDuffie 1986)
  938* (shake flask-surface tension measurement, measured range 10–35°C Thomsen 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):
  0.467* (extrapolated-regression of tabulated data, temp range 108.8–294°C, Stull 1947)
  0.086 (effusion method, extrapolated-Antoine eq., Small et al. 1948)
  log (P/mmHg) = 11.26 – 4308/(T/K); temp range 32–60°C or pressure range 5 × 10⁻² to 10⁻⁴ mmHg (effusion method, data presented in graph and Antoine eq., Small et al. 1948)
  0.052 (20°C, torsion-effusion method, Balson 1958)
  0.0195 (20°C, aerosol saturation, measured range 25–70°C, Frostling 1970)
  log (P/mmHg) = 11.13 – 4275/(T/K); temp range 25–70°C (aerosol saturation, Frostling 1970)
  0.467 (calculated-Antoine eq., Weast 1972–73)
  log (P/mmHg) = [−0.2185 × 15383.0/(T/K)] + 8.18275; temp range 108.8–294°C (Antoine eq., Weast 1972–73)
Esters 3085

0.046* (20°C, extrapolated, gas-saturation method, measured range 34.2–60.5°C, Grayson & Fosbraey 1982)
\ln (P/Pa) = 32.50 – 10436/(T/K); temp range 34.2–60.5°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)

1.867 (gas saturation, measured range 60–120°C. Potin-Gautier et al. 1982)
\log (P/mmHg) = 8.806 – 1443.039/(T/K); temp range 60–120°C (Potin-Gautier et al. 1982)

0.220 (gas saturation-HPLC/UV, Howard et al. 1985)
0.0064 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
\log (P/kPa) = 6.04308 – 1866.05/(–115.9 + T/K); temp range 345–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)

1.867 (gas saturation-GC, Grayson & Fosbraey 1982)
\log (P/mmHg) = 8.806 – 1443.039/(T/K); temp range 60–120°C (Potin-Gautier et al. 1982)

Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0020 (calculated-P/C, Wolfe et al. 1980a)
0.0486 (Lyman et al. 1982; quoted, Howard 1989)
0.1220 (calculated-P/C, Mabey et al. 1982)
4.7100 (quoted from WERL Treatability Data, Ryan et al. 1988)
0.0269 (selected, Staples et al. 1997)

Octanol/Water Partition Coefficient, log K_{OW}:
3.22 (calculated as per Leo et al. 1971)
3.15 (RP-HPLC-RT correlation, Veith et al. 1979)
1.40 (shake flask-LSC, Veith et al. 1980)
2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
2.21 (HPLC-RT correlation, McDuffie 1981)
2.70 (quoted from Veith et al. 1980, Veith & Kosian 1983; Davies & Dobbs 1984; Saito et al. 1992)
2.35 (20°C, shake flask-UV, Leyder & Boulanger 1983)
2.24, 2.29 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)
2.47 (shake flask, unpublished data, Hansch & Leo 1985; 1987)
3.00 (RP-HPLC-RT correlation, De Koch & Lord 1987)
2.47 (recommended, Sangster 1993)
2.47 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
7.55 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:
0.49–1.56 (calculated-K_{OW}, Veith et al. 1979, 1980)
2.07 (bluegill sunfish, Veith et al. 1980; Barrows et al. 1980; Veith & Kosian 1983)
1.86 (bacteria, calculated-K_{OW}, Wolfe et al. 1980a)
1.08, 1.64 (calculated-S, calculated-K_{OW}, Lyman et al. 1982)
2.04 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.19 (mullet, Shimada et al. 1983)
2.10 (Davies & Dobbs 1984)
2.07 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.65 (calculated-K_{OW}, Wolfe et al. 1980a)
2.72 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)
1.97 (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)
2.15 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct $k_P = 2 \times 10^{-4}$ h$^{-1}$ (EXAMS model, Wolfe et al. 1980a)

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

$\kappa$(aq.) = 18 M s$^{-1}$ in aquatic environment (Wolfe et al. 1980a)

$k << 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 1.4$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}} = 1.08 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ corresponding to $t_{1/2} = 22.2$ h and the alkyl peroxy reaction $t_{1/2}(\text{calc}) = 6.5$ yr (Howard 1989)

photooxidation $t_{1/2} = 21$–212 h in air, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photooxidation $t_{1/2} = 2.4$–12.2 yr in water, based on estimated rate data for the reaction with alkylperoxyl radical in aqueous solution (Howard et al. 1991)

$k$(aq.) = $(0.14 \pm 0.05) \times 10^{-2}$ M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 2.8$ d at pH 7 (Yao & Haag 1991).

$k_{\text{OH}}(\text{aq.}) = 4 \times 10^{-9}$ M$^{-1}$ s$^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

predicted atmospheric photooxidation $t_{1/2} = 1.8$–18 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{\text{OH}} = 3.466 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $t_{1/2} = 2.39$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: $k$(acid-catalyzed) = 0.04 M$^{-1}$ h$^{-1}$, $k$(alkaline) = 79 M$^{-1}$ h$^{-1}$; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ months to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

$k$(second-order alkaline) = $2.5 \times 10^{-2}$ M$^{-1}$ s$^{-1}$ at 30°C (Wolfe et al. 1980b; quoted, Kollig 1993)

$k$(alkaline) = $2.5 \times 10^{-2}$ M$^{-1}$ s$^{-1}$ at 30°C and $k$(second-order alkaline rate) = $1.2 \times 10^{-2}$ M$^{-1}$ s$^{-1}$ at pH 10–12 at 30°C, with a calculated $t_{1/2} = 18.3$ yr at pH 7 (Callahan et al. 1979)

First order hydrolysis $t_{1/2} = 8.8$ yr based on base rate constant at 30°C and pH 7; base rate constant $k = 90$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 32$ d based on measured rate constant at 30°C and pH from 10 to 12 (Howard et al. 1991)

$t_{1/2} = 3200$ d, $t_{1/2} = 0.032$ d in natural waters (Capel & Larson 1995)

First-order hydrolysis $t_{1/2} = 8.8$ yr at pH 7 and $t_{1/2} = 32$ d at pH 10–12 based on base rate constant at 30°C (Howard et al. 1991; selected, Staples et al. 1997)

Biodegradation: microbial degradation $t_{1/2} = 10.5$ d by microorganisms isolated from soil and waste water at 30°C (Kurane et al. 1977, quoted; Russell et al. 1985); estimated rate constant $k = (6.59 \pm 0.43) \times 10^2$ min$^{-1}$ from retention times of reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O’Grady et al. 1985);

microbial degradation $k = 2 \times 10^{-4}$ h$^{-1}$ in an aquatic environment (Wolfe et al. 1980a);

0 to 32% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

complete degradation in 7.0 d for 5 and 10 ppm DEP in domestic waste water under aerobic conditions at 25°C (Tabak et al. 1981; quoted, Howard 1989);

$k = 0.315$ d$^{-1}$ corresponding to $t_{1/2} = 2.21$ d with a mixed microbial population and underwent > 99% degradation in 28-d in shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% of DEP was degraded within 40 d in digested sludge (Shelton et al. 1984); 85% biodegraded after 14 d incubation in aerobic freshwater sediments at 22°C (Johnson et al. 1984);

biodegraded in excess of 90% in less than 24 h in activated sludge systems (O’Grady et al. 1985);
soil-water biodegradation studies showed the 86% loss after 120 h in Broome County soils and 67% loss in leachate sprayed soil after 48 h (Russell et al. 1985);
anaerobic digestion of sludge with first-order $k = 6.0 \times 10^{-3}$ h$^{-1}$ and $t_{1/2} = 115$ h (Ziogou et al. 1989)
aqueous aerobic $t_{1/2} = 72–1344$ h, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672–5376$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and anaerobic screening test data (Howard et al. 1991)
$t_{1/2}$(aerobic) = 3 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)

Aerobic biodegradation in aquatic environments, first order $k = 1.8$ d$^{-1}$ with $t_{1/2} = 0.39$ d in river water,
$k = 0.16$ d$^{-1}$ with $t_{1/2} = 4.33$ d in MITI inoculum, and $k = 0.98$ d$^{-1}$ with $t_{1/2} = 0.71$ d (Peterson & Staples 2003)
biodegradation in aerobic soil, pseudo-first-order $k = 0.38$ d$^{-1}$ with $t_{1/2} = 1.83$ d in agitated aqueous suspension.

For anaerobic degradation, first order rate $k = 0.069$ to > 0.3 d$^{-1}$ with $t_{1/2} = 10.0$ to < 2.3 d in digester sludge, batch incubation; $k = 0.036$ d$^{-1}$ with $t_{1/2} = 19.3$ d in flood soil; $k = 0.27$ d$^{-1}$ with $t_{1/2} = 2.6$ d in pond sediment, $k = 0.13$ d$^{-1}$ with $t_{1/2} = 5.3$ d in 10% freshwater sediment and $k = 0.31$ d$^{-1}$ with $t_{1/2} = 2.2$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: experimentally determined microbial $k = 3.2 \times 10^{-9}$ mL organism$^{-1}$ h$^{-1}$ (Wolfe et al. 1980a,c);
estimated $k \sim 1 \times 10^{-7}$ mL cell$^{-1}$ h$^{-1}$ for bacterial transformation in water (Mabey et al. 1982);
mean microbial $k = (7.2 \pm 15.4) \times 10^{-7}$ mL cell$^{-1}$ h$^{-1}$ for 54 batch aufwuchs cultures (Lewis & Holm 1981; Lewis et al. 1984).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:
depuration half-life 24 h < $t_{1/2} < 48$ h in tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 6.83$ d$^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)
$k_2 = 0.584$ d$^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: an estimated $t_{1/2} = 22.2$ h for the vapor reaction with photochemically generated $8 \times 10^3$ molecules cm$^{-3}$ OH radical in air at 25°C with an estimated $k \sim 1.08 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Howard 1989);
$t_{1/2} = 21–212$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)
photodegradation $t_{1/2} = 2.39$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 2.21$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984);
$t_{1/2} \sim 2$ d to > 2 wk for aerobic biodegradation in water; $t_{1/2} = 3$ d when incubated in dirty river water (Howard 1989);
overall degradation $t_{1/2} = 72–1344$ h, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991);
k(exptl) = (0.14 ± 0.5) M$^{-1}$ s$^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 2.8$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 144–2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 14$ d in freshwater sediment (Johnson et al. 1984).

Soil: degradation $t_{1/2} = 10.5$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);
$t_{1/2} = 10–50$ d via volatilization subject to plant uptake from soil (Ryan et al. 1988);
$t_{1/2} = 72–1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: 24 h < $t_{1/2} < 48$ h in tissues of bluegill sunfish (Barrows et al. 1980).
### TABLE 15.1.3.2.1
Reported vapor pressures and aqueous solubilities of diethyl phthalate at various pressures and solubilities

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
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<tbody>
<tr>
<td></td>
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<tr>
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<td>elution chromatography-UV</td>
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<tr>
<td>t/°C</td>
<td>g m⁻³</td>
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<tr>
<td>------------------</td>
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</tr>
<tr>
<td>20</td>
<td>1200</td>
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<tr>
<td>20</td>
<td>1240</td>
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<td>1160</td>
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<td>30</td>
<td>1400</td>
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<td>30</td>
<td>1340</td>
</tr>
</tbody>
</table>

\[
\ln P = A - \frac{B}{T/K}
\]

Diethyl phthalate: solubility vs. 1/T

![Graph](image)

**FIGURE 15.1.3.2.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for diethyl phthalate.
FIGURE 15.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl phthalate.
15.1.3.3 Diallyl phthalate (DAP)

Common Name: Diallyl phthalate
Synonym: DAP
Chemical Name: di(2-propenyl) phthalate, bis(2-propenyl)ester, 1,2-benzenedicarboxylic acid
CAS Registry No: 131-17-9
Molecular Formula: C_{14}H_{14}O_{4}, C_6H_4-1,2-(CO_2CHCH=CH_2)_2
Molecular Weight: 246.259
Melting Point (°C): -77 (Fishbein & Albro 1972)
Boiling Point (°C): 290 (Fishbein & Albro 1972)
Density (g/cm³ at 20°C): 1.121 (Fishbein & Albro 1972)
Molar Volume (cm³/mol):
219.7 (20°C, calculated-density)
288.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
Entropy of Fusion, ∆S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
< 100 (Fishbein & Albro 1972)
182 (20°C, shake flask-GC, Leyder & Boulanger 1983)
182; 43; 100 (recommended; calculated-QSAR, Staples 1997)
94 (calculated-UNIFAC, Thomsen et al. 1999)
156 (calculated-QSPR, Cousins & Mackay 2000)
Vapor Pressure (Pa at 25°C):
0.0213; 0.00493; 0.155 (recommended; calculated-QSAR, Staples et al. 1997)
0.0271 (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0289 (selected, Staples et al. 1997)
0.0428 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{OW}:
3.23 (shaken flask, Leyder & Boulanger 1983)
3.23 (recommended value, Sangster 1993)
3.23 (recommended, Hanesch et al. 1995)
3.23; 3.37; 3.63 (recommended; calculated-QSAR, Staples 1997)
3.61 (calculated-UNIFAC, Thomsen et al. 1999)
3.11 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log K_{OA}:
7.87 (calculated-QSPR, Cousins & Mackay 2000)
Bioconcentration Factor, log BCF:

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

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:
- Volatilization:
- Photolysis:
- Oxidation: atmospheric photooxidation $t_{1/2} = 0.04–0.4$ d (Staples et al. 1997).
- Hydrolysis:
- Biodegradation: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
- Biotransformation:
  Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
- Air: atmospheric photooxidation $t_{1/2} = 0.04–0.4$ d (Staples et al. 1997).
- Surface water:
- Groundwater:
- Sediment:
- Soil: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
- Biota:
### 15.1.3.4 Di-n-propyl phthalate (DnPP)

![Chemical Structure of Di-n-propyl phthalate](image)

- **Common Name:** Di-n-propyl phthalate
- **Synonym:** DPP, DNPP, dipropyl phthalate
- **Chemical Name:** phthalic acid dipropyl ester; 1,2-benzenedicarboxylic acid dipropyl ester
- **CAS Registry No:** 131-16-8
- **Molecular Formula:** C\textsubscript{14}H\textsubscript{18}O\textsubscript{4}, C\textsubscript{6}H\textsubscript{4}[COOCH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{3}]\textsubscript{2}
- **Molecular Weight:** 250.291

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C):</td>
<td>–31.0 (Lide 2003)</td>
</tr>
<tr>
<td>Boiling Point (°C):</td>
<td>304.5 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm(^3) at 20°C):</td>
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</tr>
<tr>
<td>Molar Volume (cm(^3)/mol):</td>
<td>232.2 (20°C, calculated-density, Stephenson &amp; Malanowski 1987)</td>
</tr>
<tr>
<td></td>
<td>302.8 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, ∆H\textsubscript{v} (kJ/mol):</td>
<td>88.70 (Small et al. 1948)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ∆H\textsubscript{fus} (kJ/mol):</td>
<td></td>
</tr>
<tr>
<td>Entropy of Fusion, ∆S\textsubscript{fus} (J/mol K):</td>
<td></td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ∆S\textsubscript{fus} = 56 J/mol K), F:</td>
<td>1.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Solubility (g/m(^3) or mg/L at 25°C):</td>
<td>108 (shake flask-UV, Leyder &amp; Boulanger 1983)</td>
</tr>
<tr>
<td></td>
<td>108; 38, 47 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)</td>
</tr>
<tr>
<td></td>
<td>77 (calculated-QSPR, Cousins &amp; Mackay 2000)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C and reported temperature dependence equations):</td>
<td>0.0175 (effusion method, extrapolated-Antoine eq., Small et al. 1948)</td>
</tr>
<tr>
<td></td>
<td>log (P/mmHg) = 11.66 – 4634/(T/K); temp range 32–75°C or pressure range 5 × 10(^{-2}) to 10(^{-4}) mmHg (Antoine eq., effusion method, Small et al. 1948). Additional data at other temperatures designated * are compiled at the end of this section</td>
</tr>
<tr>
<td></td>
<td>log (P/kPa) = 8.625 – 3824/(T/K); temp range 403–578 K (Antoine eq., Stephenson &amp; Malanowski 1987)</td>
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<td>0.0119, 0.138 (calculated-QSAR, Staples et al. 1997)</td>
</tr>
<tr>
<td></td>
<td>0.0175 (calculated-QSPR, Cousins &amp; Mackay 2000)</td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa·m(^3)/mol at 25°C):</td>
<td>0.0309 (recommended, Staples et al. 1997)</td>
</tr>
<tr>
<td></td>
<td>0.0569 (calculated-QSPR, Cousins &amp; Mackay 2000)</td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log K\textsubscript{ow}:</td>
<td>3.27 (shake flask, Leyder &amp; Boulanger 1983)</td>
</tr>
<tr>
<td></td>
<td>4.05 (HPLC-RT correlation, Hayward et al. 1990)</td>
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<td>4.20 (HPLC-RT correlation, Jenke et al. 1990)</td>
</tr>
<tr>
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<td>3.27, 4.05 (lit. values, Hansch et al. 1995)</td>
</tr>
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<td></td>
<td>3.27; 3.57, 3.63 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)</td>
</tr>
<tr>
<td></td>
<td>3.636 (Thomsen &amp; Carlsen 1998)</td>
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<td></td>
<td>3.40 (calculated-QSPR, Cousins &amp; Mackay 2000)</td>
</tr>
</tbody>
</table>
Octanol/Air Partition Coefficient, $\log K_{OA}$:
8.04 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

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

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: atmospheric photooxidation $t_{1/2} = 0.9–9.0$ d (calculated, Staples et al. 1997).
Hydrolysis:
Biodegradation: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);
rate constant $k = (10.71 \pm 0.73) \times 10^{-2}$ min$^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).
Aerobic biodegradation in aquatic environments, first order $k = 1.3$ d$^{-1}$ with $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: atmospheric photooxidation $t_{1/2} = 0.9–9.0$ d (calculated, Staples et al. 1997).
Surface water: $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)
Groundwater:
Sediment:
Soil: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

**FIGURE 15.1.3.4.1** Logarithm of vapor pressure versus reciprocal temperature for di-$n$-propyl phthalate.
15.1.3.5 Di-isopropyl phthalate (DIPP)

Common Name: Di-isopropyl phthalate
Synonym: DIPP
Chemical Name: phthalic acid dipropyl ester, bis(1-methylethyl)ester, 1,2-benzenedicarboxylic acid didiopropy ester
CAS Registry No: 605-45-8
Molecular Formula: C_{14}H_{18}O_{4}
Molecular Weight: 250.291
Melting Point (°C): liquid
Boiling Point (°C): 304–305 (Weast 1982–83)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
302.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
322 (shake flask-UV, Leyder & Boulanger 1983)
136 (calculated-UNIFAC, Thomsen et al. 1999)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
2.83 (shake flask-UV, Leyder & Boulanger 1983)
2.83 (recommended, Sangster 1993)
2.83 (recommended, Hansch et al. 1995)
3.59 (calculated-UNIFAC, Thomsen et al. 1999)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:
Biodegradation: degradation t_{½} = 1.5 d by microorganisms (Pseudomonas acidovorans 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
Half-Lives in the Environment:
Soil: degradation t_{½} = 1.5 d by microorganisms (Pseudomonas acidovorans 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
15.1.3.6 Di-n-butyl phthalate (DBP)

![Chemical Structure](image)

Common Name: Dibutyl phthalate
Synonym: n-butyl phthalate, di-n-butyl phthalate, DBP, dibutyl o-phthalate, o-benzenedicarboxylic acid dibutyl ester, benzene-o-dicarboxylic acid dibutyl ester
Chemical Name: phthalic acid dibutyl ester, di-n-butyl phthalate
CAS Registry No: 84-74-2
Molecular Formula: C_{16}H_{22}O_{4}, o-C_{6}H_{4}(COOC_{4}H_{9})_{2}
Molecular Weight: 278.344
Melting Point (°C):
-35.0 (Fishbein & Albro 1972; Verschueren 1977, 1983; Dean 1985; Howard 1989; Lide 2003)
Boiling Point (°C):
340.0 (Stull 1947; Fishbein & Albro 1972; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
1.0465 (21°C, Fishbein & Albro 1972)
1.047 (Weast 1982–83)
Molar Volume (cm³/mol):
267.1 (calculated-density, Stephenson & Malanowski 1987)
347.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
93.3 (Small et al. 1948)
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: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
11.08 (Deno & Berkheimer 1960)
4500 (Patty 1967)
4500 (Fishbein & Albro 1972)
10.0 (30°C, from Monsanto Chemical Co. data sheets, Peakall 1975)
13.0 (Wolfe et al. 1979; Wolfe et al. 1980a)
10.8, 11.1, 10.5 (20°C: quoted average, elution chromatography, UV, Schwarz & Miller 1980)
11.4, 11.5, 11.2 (30°C: quoted average, elution chromatography, UV, Schwarz & Miller 1980)
13 ± 1.6, 4.45 (shake flask-GC, quoted, Wolfe et al. 1980b; quoted, Staples et al. 1997)
3.25 (solubility in 35 liter instant ocean, Giam et al. 1980)
10.1 (20°C, shake flask-UV, Leyder & Boulanger 1983)
400, 4500 (Verschueren 1983)
28.0 (26°C, Verschueren 1983)
11.2 ± 0.3 (shake flask-HPLC/UV, Howard et al. 1985)
100 (Dean 1985)
11.2 (Howard et al. 1985)
9.40 (best estimate by turbidity inflection, DeFoe et al. 1990)
8.70, 9.40 (centrifugation-HPLC/UV, turbidity inflection-HPLC/UV, DeFoe et al. 1990)
11.2 (recommended, Staples et al. 1997)
9.90 (calculated-QSPR, Cousin & Mackay 2000)
13.3, 14.6, 5.50 (10, 25, 35°C, shake flask-surface tension measurement, Thomsen et al. 2001). Additional data at other temperatures designated * are compiled at the end of this section
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):

13.33* (89°C, ebulliometry, measured range 89–176°C, Gardner & Brewer 1937)
0.00233 (20°C, extrapolated, tensimeter, measured range 52–97°C, Hickman et al. 1937)

\[ \log(P/\mu \text{mHg}) = 14.215 - 4680/(T/\text{K}) \; \text{ temp range 52–97°C} \; \text{Hickman et al. 1937} \]

0.0171* (20°C, extrapolated, effusion, measured range 40–95°C, Verhoek & Marshall 1939)

\[ \log(P/\mu \text{mHg}) = 15.589 - 5122/(T/\text{K}) \; \text{ temp range 40–95°C} \; \text{Verhoek & Marshall 1939} \]

0.00253* (ebulliometry, extrapolated from graph, measured range 50–172°C, Burrows 1946)

0.0217* (extrapolated-regression of tabulated data, temp range 148.2–340°C, Stull 1947)

0.00345, 0.0043 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

\[ \log(P/\mu \text{mHg}) = 11.75 - 4450/(T/\text{K}) \; \text{ temp range 55–102°C} \; \text{Perry & Weber 1949} \]

0.00364* (effusion method, measured range 19.9–44°C, Birks & Bradley 1949)

7.6 × 10⁻⁵ (dew-point method and tensimeter method, temp range of 72–185°C, extrapolated-Antoine eq., Werner 1952)

log (P/mmHg) = 11.008 – 2872/(T/°C); temp range 72–185°C (Antoine eq., from transpiration-GC measurement, Hales et al. 1981)

0.0027 (20°C, transpiration-GC “collection” measurement, Hales et al. 1981)

0.0011 (saturated column-HPLC/UV, Howard et al. 1985)

0.00355 (extrapolated, Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log(P/\mu \text{mHg}) = 152.675 - 1.0754 \times 10^4/(T/\text{K}) – 51.17 \log(T/\text{K}) + 1.6933 \times 10^{-2}(T/\text{K}) + 2.4948 \times 10^{-14}(T/\text{K})^2 \; \text{ temp range 238–781 K} \; \text{Yaws et al. 1994} \]

0.0027 (liquid P, GC-RT correlation, Donovan 1996)
Esters

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

- 0.1320 (calculated-P/C, Wolfe et al. 1980a)
- 0.0466 (Lyman et al. 1982; quoted, Howard 1989)
- 0.0284 (calculated-P/C, Mabey et al. 1982)
- 0.1835 (Atlas et al. 1983)
- 0.456, 0.446 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
- 0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 0.0895 (selected, Staples et al. 1997)
- 0.133 (calculated-QSPR, Cousins & Mackay 2000)

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

- 5.20 (calculated as per Leo et al. 1971, Callahan et al. 1979)
- 5.15 (RP-HPLC-RT correlation, Veith et al. 1979)
- 4.13 (HPLC-RT correlation, McDuffie 1981)
- 4.11, range 3.23–4.45 (shake flask-concn ratio, OECD 1981)
- 4.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
- 4.39, 4.56 (HPLC-extrapolated, Harnish et al. 1983)
- 4.57 (20°C, shake flask-UV, Leyder & Boulanger 1983)
- 4.79, 3.74 (shake flask-HPLC/UV, HPLC-RT, Howard et al. 1985)
- 4.11 (OECD value, Howard et al. 1985)
- 4.72 (shake flask, Hansch & Leo 1985; 1987)
- 4.57 (HPLC-k correlation, Eadsforth 1986)
- 4.30 (HPLC-RT correlation, Haky & Leja 1986)
- 4.72 (measured value, DeFoe et al. 1990)
- 4.72 (recommended, Sangster 1993)
- 4.72 (recommended, Hansch et al. 1993)
- 4.01 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schränder 1999)

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

- 8.54 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

- 3.15 (fish, Mayer & Sanders 1973)
- 3.82, 3.70, 3.83, 3.28, 3.70, 3.43 (midge larvae, waterflea, scud, mayfly, grass shrimp, damselfly, Sanders et al. 1973)
- 3.83 (fish, Sanders et al. 1973)
- 1.32 (calculated, Kenaga 1980)
- 3.90 (bacteria, calculated-$K_{ow}$, Wolfe et al. 1980a)
- 1.32–1.62, 0.46–1.49, 1.07 (oyster, shrimp, fish, Wofford et al. 1981)
- 1.50, 1.22, 1.07 (American oyster, brown shrimp, sheehead minnow, Wofford et al. 1981)
- 4.67 (microorganisms-water, calculated-$K_{ow}$, Mabey et al. 1982)
- 4.36 ($Selenastrum capricornutum$, Casserly et al. 1983)
- 1.32 (oyster, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
- 3.68, 3.68 (oyster, estimated values, Zaroogian et al. 1985)
- 1.08 (fish, highest BCF, Matthissen et al. 1992)

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

- 2.20 (soil, estimated-S, Kenaga 1980)
- 3.81 (soil, estimated-S, Wolfe et al. 1980a)
- 2.17 (marine sediment/seawater with 1% organic carbon, Bouwer et al. 1981)
- 1.60, 1.30, 0.602 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 3–4 ppm, Sullivan et al. 1981)
Environmental Fate Rate Constant, k, and Half-Lives, t_{1/2}:

Volatilization: \( t_{1/2} = 28 \text{ d} \) from a stirred seawater solution 1.0 m deep (Atlas et al. 1982; quoted, Howard 1989)
evaporation rate \( k = 3.42 \times 10^{-10} \text{ mol cm}^{-2} \text{ h}^{-1} \) at 20°C (Gückel et al. 1982);

\( t_{1/2} \approx 47 \text{ d} \) in a river of 1.0 m deep with 1 m/s current and a 3 m/s wind using Henry’s law constant while the rate of volatilization being controlled by the diffusion through air (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: direct photolysis (near surface) rate constant \( k \approx 2 \times 10^{-4} \text{ h}^{-1} \) in natural water (Wolfe et al. 1980a)
aqueous photolysis rate \( k = 0.23 \text{ h}^{-1} \) and \( t_{1/2} = 3 \text{ h} \) (Jin et al. 1999, quoted, Peterson & Staples 2003)
Indirect photolysis \( k = 0.29 \text{ d}^{-1} \) with \( t_{1/2} = 2.4 \text{ d} \) in air (Peterson & Staples 2003).

Oxidation:
\( k = 18 \text{ M s}^{-1} \), the free radical oxidation rate constant (EXAMS model, Wolfe et al. 1980a)
photooxidation \( t_{1/2} = 2.4–12.2 \text{ yr} \) in water, based on estimated rate data for the reaction with alklyloxyl radical in aqueous solution (Wolfe et al. 1980a; quoted, Howard et al. 1991)
\( k << 360 \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and \( k = 1.4 \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical (Mabey et al. 1982)
photooxidation \( t_{1/2} = 18.4 \text{ h} \) with reaction with OH radical (Howard 1989)
photooxidation \( t_{1/2} = 7.4–74 \text{ h} \) in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Atmospheric photooxidation \( t_{1/2} = 0.6–6.0 \text{ d} \) from Atkinson 1988 atmospheric-oxidation program (estimated, Staples et al. 1997).

\( k_{\text{OH}} = 9.277 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) and \( t_{1/2} = 0.89 \text{ d} \) based on a global, seasonal and diurnal average OH radical concn of 1 \times 10^6 \text{ molecule cm}^{-3} \) in air (Peterson & Staples 2003)

Hydrolysis:
\( k(\text{second-order alkaline}) = 2.2 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1} \) for pH 10–12 at 30°C, with calculated half-life of 10 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)
\( k(\text{acid catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1} \), \( k(\text{second order alkaline}) = 38 \text{ M}^{-1} \text{ h}^{-1} \) in an aquatic environment (Wolfe et al. 1980a)
\( k(\text{second-order alkaline}) = (1.0 \pm 0.05) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1} \) at pH 7 and 30°C, with first-order hydrolysis \( t_{1/2} = 10 \text{ yr} \) (Wolfe et al. 1980b; quoted, Kollig 1993);

\( t_{1/2} = 76 \text{ d} \) at pH 9 and \( t_{1/2} = 10 \text{ yr} \) at neutral pH (estimated, Howard 1989)
\( t_{1/2} = 10 \text{ yr} \), based on the overall hydrolysis rate constant (Howard et al. 1991)
aqueous abiotic \( t_{1/2} = 22 \text{ yr} \) (selected, Staples et al. 1997)
\( t_{1/2} = 3700 \text{ d} \) at pH 7, \( t_{1/2} = 76 \text{ d} \) at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation:
\( t_{1/2} = 3 \text{ d} \) by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
DBP was rapidly degraded, 3% left after 5 d, but under anaerobic conditions required 30 d for the degradation
freshwater hydrosoil, under aerobic conditions (Johnson et al. 1979, quoted, Russell et al 1985)
a 90% loss in 3 d from river water (Brinkman et al. 1979, quoted, Russell et al. 1985)
\( k = (13.26 \pm 0.73) \times 10^7 \text{ min}^{-1} \) (reversed phase-GC-RT correlation, Urushigawa & Yonezawa 1979; quoted, O’Grady et al. 1985)
\( k = 2.9 \times 10^{-8} \text{ mL organism}^{-1} \text{ h}^{-1} \) (Wolfe et al. 1980a);
\( k > 0.5 \text{ d}^{-1} \), significant degradation with rapid adaptation within 7 d in an aerobic environment (Tabak et al. 1981; quoted, Mills et al. 1982);
\( k = 7.4 \times 10^{-7} \text{ mL cell}^{-1} \text{ d}^{-1} \) (river die-away test, Scow 1982);
32–85% degraded after 2–3 wk in municipal digested sludge (Horowitz et al. 1982)
decomposed within 80 d under both aerobic and anaerobic conditions when approximately 90% added to
soils (Inman et al. 1984)

\[
k = (0.1–7.6) \times 10^{-4} \, h^{-1} \text{ to } (4.9–36.5) \times 10^{-4} \, h^{-1} \text{ for water and water/sediment systems (under sterile condi-
tions); and } k = (29.3–409) \times 10^{-4} \, h^{-1} \text{ to } (38.2–456) \times 10^{-4} \, h^{-1} \text{ for water and water/sediment systems (under active conditions) samples from six estuarine and freshwater sites, actual } t_{1/2} = 1.0–4.8 \, d \text{ for active sediment treatment, } t_{1/2} = 1.7–13.0 \, d \text{ for active water treatment and } t_{1/2} = 8–23 \, d \text{ for sterile sediment (Walker et al. 1984)}
\]

\[
k = 0.050 \, d^{-1} \text{ and a } t_{1/2} = 15.4 \, d \text{ in a shake flask biodegradation experiment (Sugatt et al. 1984)}
\]

> 90% of DBP was degraded within 40 d in digested sludge (Shelton et al. 1984)

> 90% biodegraded in less than 24 h in activated sludge systems (O’Grady et al. 1985)

> 90% biodegraded in less than 24 h in activated sludge systems (O’Grady et al. 1985)

> 90% biodegraded in less than 24 h in activated sludge systems (O’Grady et al. 1985)

81% loss in Broome County soils after 24 h and 70% loss in leachate sprayed soil after 24 h in soil-water
biodegradation studies (Russell et al. 1985);

\[
t_{1/2} = 24–552 \, h, \text{ aqueous aerobic based on unacclimated aerobic river die-away test and soil grab sample data}
\]

\[
t_{1/2} = 48–552 \, h, \text{ aqueous anaerobic, based on unacclimated anaerobic grab sample data for soil and sediment}
\]

(Biolk & Lulves 1975; Verschueren 1983; Howard et al. 1991)

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

\[
k = 0.0216 \, h^{-1} \text{ with } t_{1/2} = 32.1 \, h \text{ for microbial degradation by anaerobic sludge (Wang et al. 2000)}
\]

\[
\text{biodegradation in aerobic environments, first order } k = 0.8 \, d^{-1} \text{ with } t_{1/2} = 0.87 \, d \text{ in river water, } k = 0.51 \, d^{-1} \text{ with } t_{1/2} = 1.56 \, d \text{ in estuarine and river water, } k = 0.29 \, d^{-1} \text{ with } t_{1/2} = 2.40 \, d \text{ in sediment microcosm,}
\]

\[
k = 0.22 \, d^{-1} \text{ with } t_{1/2} = 3.15 \, d \text{ in MITI inoculum, } k = 0.14 \, d^{-1} \text{ with } t_{1/2} = 4.95 \, d \text{ in river water, low sediment,}
\]

\[
k = 0.98 \, d^{-1} \text{ with } t_{1/2} = 0.71 \, d \text{ river water only (Peterson & Staples 2003)}
\]

\[
bioconcentration, \text{ Uptake (} k_1 \text{) and Elimination (} k_2 \text{) Rate Constants or half-Lives:}
\]

\[
t_{1/2} = 3 \, d \text{ in } Daphnia magna (Mayer & Sanders 1973).
\]

\[
k_2 = 0.237 \, d^{-1} \text{ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)}
\]

\[
k_2 = 0.0114 \, d^{-1} \text{ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)}
\]

Half-Lives in the Environment:

Air: \( t_{1/2} \approx 18 \, h \) for the vapor phase reaction with hydroxyl radicals in air (Howard 1989);

\[
t_{1/2} = 7.4–74 \, h \text{ based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)};
\]

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

Photodegradation \( t_{1/2} = 0.89 \, d \text{ based on a global, seasonal and diurnal average OH radical concn of } 1 \times 10^6 \text{ molecule cm}^{-3} \text{ in air and indirect photolysis } t_{1/2} = 2.4 \, d \text{ (Peterson & Staples 2003)}
\]

Surface water: biodegradation \( t_{1/2} = 15.4 \, d \text{ in an acclimated shake flask CO}_2 \text{ evolution test (Sugatt et al. 1984)}
\]

\[
t_{1/2} = 2–12 \, d \text{ in water alone (Howard 1989)};
\]

\[
t_{1/2} = 24–336 \, h \text{, based on unacclimated aerobic river die-away test and fresh water/sediment grab sample}
\]

\[
data (Howard et al. 1991)
\]

Biodegradation \( t_{1/2}(aerobic) = 1 \, d, \text{ } t_{1/2}(anaerobic) = 2 \, d \); hydrolysis \( t_{1/2} = 3700 \, d \text{ at pH 7 and } t_{1/2} = 76 \, d \text{ at pH 12}
\]

in natural waters (Capel & Larson 1995)

biodegradation \( t_{1/2} = 0.87–5.78 \, d \) in aerobic aquatic environments (Peterson & Staples 2003)
Ground water: $t_{1/2} = 48–552\text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: 97% degradation in 5 d in an aerobic pond water-sediment mixture; $t_{1/2} = 7–30\text{ d}$ under anaerobic conditions, $t_{1/2} = 1–5\text{ d}$ in sediment-water systems of estuarine and freshwater sites (Howard 1989).

Soil: degradation $t_{1/2} = 3\text{ d}$ by microorganisms isolated from soil or waste water at $30^\circ\text{C}$ (Kurane et al. 1977);
biodegradation $t_{1/2}(\text{aerobic}) < 5\text{ d}$ and $t_{1/2}(\text{anaerobic}) \sim 20\text{ d}$ in a garden soil (Shanker et al. 1985);
overall $t_{1/2} = 48–552\text{ h}$, based on unacclimated aerobic soil grab sample data (Howard et al. 1991).

Aerobic biodegradation in soil, $t_{1/2}$ ranging from 0.43 to 19.8 d in aqueous suspension, garden soil and soils with different organic carbon contents (Peterson & Staples 2003).

Biota: elimination $t_{1/2} = 3\text{ d}$ for waterfleas *Daphnia magna* (Mayer & Sanders 1973).

---

**TABLE 15.1.3.6.1**

Reported vapor pressures of di-*n*-butyl phthalate at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\log P = A - B/(T/K) - C/(T/K)^2 \quad (5)$$

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<th>P/Pa</th>
<th>T/°C</th>
<th>P/Pa</th>
<th>T/°C</th>
<th>P/Pa</th>
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**FIGURE 15.1.3.6.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for di-*n*-butyl phthalate.
TABLE 15.1.3.6.1 (Continued)

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TABLE 15.1.3.6.1 (Continued)

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3.

Hales et al. 1981

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FIGURE 15.1.3.6.2 Logarithm of vapor pressure versus reciprocal temperature for di-\textit{n}-butyl phthalate.
15.1.3.7 Di-isobutyl phthalate (DIBP)

Common Name: Di-isobutyl phthalate  
Synonym: DIBP  
Chemical Name: phthalic acid diisobutyl ester, bis(2-methylpropyl)ester, 1,2-benzenedicarboxylic acid  
CAS Registry No: 84-69-5  
Molecular Formula: C_{16}H_{22}O_{4}  
Molecular Weight: 278.344  
Melting Point (°C):  
–58 (Staples et al. 1997)  
Boiling Point (°C):  
296.5 (Lide 2003)  
Density (g/cm³ at 20°C):  
1.040 (Fishbein & Albro 1972)  
1.049 (15°C, Weast 1982–83)  
Molar Volume (cm³/mol):  
347.2 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
100 (Fishbein & Albro 1972)  
6.20 (shake flask-nephelometry, Hollifield 1979)  
20.3 (Leyder & Boulanger 1983)  
20.0; 5.1, 9.6 (recommended; calculated-QSAR, Staples et al. 1997)  
21.6 (calculated-UNIFAC, Thomsen et al. 1999)  
9.90 (calculated-QSPR, Cousins & Mackay 2000)  
Vapor Pressure (Pa at 25°C):  
2.4 × 10⁻³, 0.0773 (calculated-QSAR, Staples et al. 1997)  
0.00473 (calculated-QSPR, Cousins & Mackay 2000)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
0.0185 (recommended, Staples et al. 1997)  
0.133 (calculated-QSPR, Cousins & Mackay 2000)  
Octanol/Water Partition Coefficient, log K_{OW}:  
4.11 (shake flask, Leyder & Boulanger 1983)  
4.43 (calculated-QSAR, Matthiessen et al. 1992)  
4.11 (quoted and recommended, Sangster 1993)  
4.11 (recommended, Hansch et al. 1995)  
4.11; 4.31, 4.46 (recommended; calculated-QSAR, Staples et al. 1997)  
4.46 (calculated-UNIFAC, Thomsen et al. 1999)  
4.27 (calculated-QSPR, Cousins & Mackay 2000)  
Bioconcentration Factor, log BCF:  
3.10 (calculated-QSAR, fish, Matthiessen et al. 1992)
Sorption Partition Coefficient, log $K_{OC}$:
- 3.14 (calculated-QSAR MCI $\chi$, Sabljic et al. 1995)
- 3.01 (suspended solids, Staples et al. 1997)

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

Volatilization:

Photolysis:
- Oxidation: atmospheric photooxidation $t_{1/2} = 0.6–6.0$ d (calculated, Staples et al. 1997)

$$k_{OH} = 9.280 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } t_{1/2} = 0.89 \text{ d based on a global, seasonal and diurnal average OH radical concn of } 1 \times 10^6 \text{ molecule cm}^{-3} \text{ in air (Peterson & Staples 2003).}$$

Hydrolysis:
- $k$(second-order alkaline) = $(1.4 - 0.2) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C in water (Wolfe et al. 1980b)

Biodegradation: degradation $t_{1/2} = 3.0$ d by microorganisms ($Pseudomonas acidovorans$ 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

- Aerobic biodegradation in aquatic environments, first order $k = 0.8$ d$^{-1}$ with $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
- $k_2 = 0.134$ d$^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)
- $k_2 = 0.0114$ d$^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

- Air: atmospheric photooxidation half-life of 0.6–6.0 d (calculated, Staples et al. 1997).

- photodegradation $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

- Surface water: biodegradation $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

Groundwater:

- Sediment:

Soil: degradation $t_{1/2} = 3.0$ d by microorganisms ($Pseudomonas acidovorans$ 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:
15.1.3.8 Dipentyl phthalate (DPP)

Common Name: Dipentyl phthalate
Synonym: DPeP, di-\(n\)-amyl phthalate
Chemical Name: dipentyl phthalate, phthalic acid diphenyl ester, 1,2-benzenedicarboxylic acid diphenyl ester
CAS Registry No: 131-18-0
Molecular Formula: \( \text{C}_{18}\text{H}_{26}\text{O}_{4} \)
Molecular Weight: 306.397
Melting Point (°C):
\(< –54.5 \) (Stephenson & Malanowski 1987)
Boiling Point (°C):
342 (Stephenson & Malanowski 1987)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
299.8 (16°C, Stephenson & Malanowski 1987)
391.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
99.16 (Small et al. 1948)
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.082 (shake flask-nephelometry, Hollifield 1979)
0.1–0.8 (shake flask-GC, Leyder & Boulanger 1983)
0.522, 1.69 (quoted, calculated-UNIFAC, Thomsen et al. 1999)
1.30 calculated-QSPR, Cousins & Mackay 2000)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.68 × 10⁻⁴ (effusion method, extrapolated-Antoine eq., Small et al. 1948)
\( \log (P/\text{mmHg}) = 12.04 – 5191/(T/K) \); temp range 55–102°C or pressure range 5 × 10⁻² to 10⁻⁴ mmHg (Antoine eq., effusion, data presented in graph, Small et al. 1948) (See figure at the end of this section.)
0.0014 (20°C, extrapolated, tensimeter, measured range 63–111°C, Perry & Weber 1949)
\( \log (P/\mu\text{mHg}) = 13.57 – 4560/(T/K) \); temp range 63–111°C (pendulum-tensimeter method, Perry & Weber 1949)
5.68 × 10⁻⁴ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\( \log (P/\text{kPa}) = 11.165 – 5191/(T/K) \); temp range 303–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
0.00128 (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.302 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):
5.33 (calculated-UNIFAC, Thomsen et al. 1999)
5.12, 5.62 (calculated-QSPR, quoted lit., Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log $K_{OA}$:

9.03 (calculated-QSPR, Cousins & Mackay 2000)

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:
Hydrolysis:
Biodegradation: degradation $t_\text{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);
rate constant $k = (9.12 \pm 1.51) \times 10^{-2}$ min$^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).
aerobic biodegradation in aquatic environments, first order $k = 1.3$ d$^{-1}$ with $t_\text{1/2} = 5.3$ d in river water (Peterson & Staples 2003)
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: biodegradation $t_\text{1/2} = 5.3$ d in aerobic aquatic environments (Peterson & Staples 2003)
Groundwater:
Sediment:
Soil: degradation $t_\text{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
Biota:

FIGURE 15.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for dipentyl phthalate.
15.1.3.9  Di-\textit{n}-hexyl phthalate (DHP)

![Chemical Structure of Di-n-hexyl phthalate](image)

Common Name: Di-\textit{n}-hexyl phthalate
Synonym: DHP, DnH(6)P
Chemical Name: Di-\textit{n}-hexyl phthalate, dihexyl ester, 1,2-benzenedicarboxylic acid
CAS Registry No: 84-75-3, 68515-50-4
Molecular Formula: C\textsubscript{20}H\textsubscript{30}O\textsubscript{4}, C\textsubscript{6}H\textsubscript{4}[COOCH\textsubscript{2}(CH\textsubscript{2})\textsubscript{4}CH\textsubscript{3}]\textsubscript{2}
Molecular Weight: 334.450
Melting Point (°C):

-27.4  (Staples et al. 1997)

Boiling Point (°C):

Density (g/cm\textsuperscript{3} at 20°C):

0.990  (Fishbein & Abro 1972)

Molar Volume (cm\textsuperscript{3}/mol):

227.8  (20°C, calculated-density)

436.0  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):

102.9  (Small et al. 1948)

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\textsuperscript{3} or mg/L at 25°C or as indicated):

- insoluble  (Fishbein & Abro 1972)
- 0.24  (shake flask-HPLC/UV, Howard et al. 1985)
- 0.05; 0.19, 0.049  (recommended; calculated-QSAR, Staples et al. 1997)
- 0.046  (shake flask-GC, Ellington 1999)
- 0.47  (calculated-UNIFAC method, Thomsen et al. 1999)
- 0.159  (calculated-QSPR, Cousins & Mackay 2000)
- 0.94, 0.52, 0.38  (10, 25, 35°C, shake flask-surface tension measurement, Thomsen et al. 2001) (See figure at the end of this section.)
- 0.070  (20°C, shake flask-GC/MS, Letinski et al. 2002)

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

\[
\log \left( \frac{P}{\text{mmHg}} \right) = 11.98 - 5381/(T/\text{K}) \quad \text{temp range 72–112°C or pressure range 5 \times 10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph, Small et al. 1948) (See figure at the end of this section.)}
\]

667  (at 210°C, Fishbein & Abro 1972)

1.03 \times 10^{-3}  (Antoine eq., interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

\[
\log \left( \frac{P}{\text{kPa}} \right) = -1.01167 - 1483.636/(T/\text{K}) \quad \text{temp range 288–303 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log \left( \frac{P}{\text{kPa}} \right) = 11.105 - 5382/(T/\text{K}) \quad \text{temp range 343–387 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)}
\]

\[
\log \left( \frac{P}{\text{kPa}} \right) = -9.785 - 4805/(T/\text{K}) \quad \text{temp range 453–533 K (Antoine eq.-III for liquid, Stephenson & Malanowski 1987)}
\]

1.90 \times 10^{-3}  (gas saturation-GC, Howard et al. 1985)

0.267  (quoted, Giam et al. 1994)

0.67; 2.53 \times 10^{-6}, 1.6 \times 10^{-3}  (recommended; calculated-QSAR, Staples et al. 1997)

0.000345  (calculated-QSPR, Cousins & Mackay 2000)
Henry's Law Constant (Pa·m³/mol at 25°C):
- 4.46 (recommended, Staples et al. 1997)
- 0.726 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 5.65–5.91 (HPLC-RT correlation, Howard et al. 1985)
- 5.80 (quoted value of Howard et al. 1985, Sangster 1993)
- 5.80 (Hansch et al. 1995)
- 6.30; 6.57, 6.67 (recommended; calculated-QSAR, Staples et al. 1997)
- 6.20 (calculated-UNFAC, Thomsen et al. 1999)
- 6.00 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log $K_{oa}$:
- 9.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{oc}$:
- 4.72 (soil/sediment, Staples et al. 1997)

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

Volatileization:

Photolysis:
- Oxidation: atmospheric photooxidation $t_{1/2} = 0.4–4.0$ d (calculated, Staples et al. 1997).

Hydrolysis:
- Biodegradation: rate constant $k = (6.86 \pm 0.23) \times 10^{-2}$ min⁻¹ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979);

Biotransformation:
- Primary biodegradation rate constant $k = 0.241$ d⁻¹ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO₂ evolution test (Sugatt et al. 1984).

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

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.4–4.0$ d (calculated, Staples et al. 1997).
- Photodegradation $t_{1/2} = 0.55$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm⁻³ in air (Peterson & Staples 2003)
- Surface water: primary biodegradation rate constant $k = 0.241$ d⁻¹ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO₂ evolution test (Sugatt et al. 1984).
FIGURE 15.1.3.9.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for dihexyl phthalate.

FIGURE 15.1.3.9.2 Logarithm of vapor pressure versus reciprocal temperature for dihexyl phthalate.
Butyl-2-ethylhexyl phthalate (BOP)

Common Name: Butyl-2-ethylhexyl phthalate
Synonym: BEHP, BOP
Chemical Name: Butyl-2-ethylhexyl phthalate
CAS Registry No: 85-69-8
Molecular Formula: C_{20}H_{30}O_{4}, (C_{4}H_{9}OOC)C_{6}H_{4}(COOCH_{2}CH(C_{2}H_{5})(CH_{2})_{3}CH_{3})
Molecular Weight: 333.450
Melting Point (°C): 
-37 (Staples et al. 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C): 
Molar Volume (cm³/mol): 446.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
< 1.0 (shake flask-HPLC/UV spec., Howard et al. 1985)
0.11; 0.02 (recommended; calculated-QSAR, Staples et al. 1997)
0.075 (calculated-UNIFAC, Thomsen et al. 1999)
0.385 (calculated-QSPR, Cousins & Mackay 2000)
Vapor Pressure (Pa at 25°C):
1.47 x 10^{-5}; 3.2 x 10^{-3}; 0.016 (recommended; calculated-QSAR, Staples et al. 1997)
5.37 x 10^{-4} (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
0.0405 (recommended, Staples et al. 1997)
0.466 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{OW}:
5.93 (av. from OECD, Howard et al. 1985)
3.70–7.88 (calculated-HPLC-RT, Howard et al. 1985)
6.28; 6.5 (recommended, calculated-QSAR, Staples et al. 1997)
6.20 (calculated-UNIFAC, Thomsen & Carlsen 1998)
5.64 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log K_{OA}:
9.37 (calculated-QSPR, Cousins & Mackay 2000)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
6.30 (suspended solids, Staples et al. 1997)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

**Volatilization:**
Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4}$ h$^{-1}$ (EXAMS model, Wolfe et al. 1980a)
Oxidation: atmospheric photooxidation $t_{1/2} = 0.4$–4.0 d (calculated, Staples et al. 1997).

**Hydrolysis:**
- $k$ (second-order alkaline) = $(1.1 \pm 0.1) \times 10^{-4}$ M$^{-1}$ s$^{-1}$ for pH 10–12 at 30°C, with $t_{1/2}$(calc) = 2000 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)
- $k$ (acid catalyzed) = 0.04 M$^{-1}$ h$^{-1}$, $k$ (second order alkaline) = 0.4 M$^{-1}$ h$^{-1}$ in an aquatic environment (Wolfe et al. 1980a)
- $k$ (second-order alkaline) = $(1.1 \pm 0.1) \times 10^{-4}$ M$^{-1}$ s$^{-1}$ at 30°C in water with $t_{1/2} = 100$–2000 yr (Wolfe et al. 1980b)

**Biodegradation:** primary biodegradation rate constant $k = 0.153$ d$^{-1}$ and $t_{1/2} = 4.55$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984)

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

**Half-Lives in the Environment:**
- Air: atmospheric photooxidation $t_{1/2} = 0.4$–4.0 d (calculated, Staples et al. 1997).
- Surface water: hydrolysis $t_{1/2} = 100$–2000 yr (Wolfe et al. 1980b; Callahan et al. 1979);
  - primary biodegradation rate constant $k = 0.153$ d$^{-1}$ and $t_{1/2} = 4.55$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).
- Groundwater:
- Sediment:
- Soil:
- Biota:
15.1.3.11 Di-\textit{n}-octyl phthalate (DOP)

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{di_n-octyl_phthalate_structure}
\caption{Structure of Di-\textit{n}-octyl phthalate (DOP)}
\end{figure}

Common Name: Di-\textit{n}-octyl phthalate

Synonym: \textit{di}-\textit{n}-octyl phthalate, DOP, \textit{o}-benzenedicarboxylic acid diocyl ester, \textit{n}-dioctyl phthalate, octyl phthalate, diocetyl-\textit{o}-benzenedicarboxylate

Chemical Name: di-\textit{n}-octyl phthalate

CAS Registry No: 117-84-0

Common Molecular Formula: C_{24}H_{38}O_4, C_6H_4(COOC_8H_{17})_2

Molecular Weight: 390.557

Melting Point (°C):
-25.0 \quad (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982; Lide 2003)

Boiling Point (°C):
220.0 \quad (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982)

Density (g/cm$^3$ at 20°C):
0.978 \quad (Fishbein & Albro 1972; Ellington 1999)

Molar Volume (cm$^3$/mol):
399.3 \quad (20°C, calculated-density)
524.8 \quad (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), $F$: 1.0

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated):
50.0 \quad (20°C, Fishbein & Albro 1972)
3.0 \quad (shake flask-GC, Wolfe et al. 1979)
3.0 \quad (shake flask-GC, Wolfe et al. 1980a,b)
0.285 \quad (24°C, tech. grade, Verschueren 1983)
0.022 \quad (generator column-HPLC/UV, DeFoe et al. 1990)
0.020, 0.040 \quad (synthesized phthalates by turbidity inflection-HPLC/UV, DeFoe et al. 1990)
1.96 \quad (calculated-molar volume, Wang et al. 1992)
0.0005 \quad (recommended, Staples et al. 1997)
0.00051; 0.00049 \quad (shake flask: slow stirring; no-stirring, GC/FID, Ellington 1999)
0.0092 \quad (calculated-UNIFAC method, Thomsen et al. 1999)
0.0249 \quad (calculated-QSPR, Cousins & Mackay 2000)
0.00040 \quad (20°C, shake flask-GC/MS, Letinski et al. 2002)
0.00040, 0.00042 \quad (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.21 \times 10^{-6} \quad (20°C, tensimeter, extrapolated, measured range 113–162°C, Perry & Weber 1949)
\log (P/\mu\text{mHg}) = 14.68 – 5620/(T/K); temp range 113–162°C (tensimeter, Perry & Weber 1949)
0.0187 \quad (estimated by analogy to Henry’s law constant, Mabey et al. 1982)
2.92 \times 10^{-5} \quad (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\log (P_p/k\text{Pa}) = 9.897 – 5197.4/(T/K), temp range: 423–523 K, (Antoine eq., Stephenson & Malanowski 1987)
1.33 \times 10^{-5} \quad (recommended, Staples et al. 1997)
2.52 \times 10^{-5} \quad (calculated-QSPR, Cousins & Mackay 2000)

Henry’s Law Constant (Pa m$^3$/mol at 25°C):
0.557 \quad (calculated-P/C, Wolfe et al. 1980a)
1.722 \quad (calculated-P/C, Mabey et al. 1982)
0.0297 \quad (quoted from WERL Treatability Data, Ryan et al. 1988)
Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:
- 9.2 (calculated as per Leo et al. 1971, Callahan et al. 1979)
- 9.2 (calculated, Wolfe et al. 1979)
- 8.06 (HPLC-RT correlation; McDuffie 1981)
- 8.92 (calculated-CLOGP for synthesized phthalate, DeFoe et al. 1990)
- 5.22 (shake flask, log P database, Hansch & Leo 1987)
- 8.06 (recommended, Staples et al. 1997)
- 6.99 (calculated-UNIFAC method, Thomsen et al. 1999)
- 7.73 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:
- 10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:
- 2.82, 3.97, 0.064, 3.72, 2.64 (in lab. model ecosystem after 3 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
- 4.45, 3.41, 3.97, 4.13 (in lab. model ecosystem after 33 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
- 3.46 (bacteria, calculated-$K_{\text{OW}}$, Wolfe et al. 1980a)
- 8.59 (microorganisms-water, calculated-$K_{\text{OW}}$, Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:
- 4.28 (calculated, Wolfe et al. 1980a)
- 9.56 (sediment-water, calculated-$K_{\text{OW}}$, Mabey et al. 1982)
- 7.91 (sediment, calculated-$K_{\text{OW}}$, Pavlou & Weston 1983, 1984)
- 7.60 (calculated-$K_{\text{OC}}$, Kollig 1993)
- 6.30 (suspended solids, calculated-$K_{d}$ assuming a 0.1 org. carbon fraction, Staples et al. 1997)

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

Volatilization:
- Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)
- Oxidation: $k = 18 \text{ M s}^{-1}$, free radical oxidation rate constant in an aquatic environment (Wolfe et al. 1980a)
- $k << 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)
- photooxidation $t_{\frac{1}{2}} = 4.5$–44.8 h in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)
- photooxidation $t_{\frac{1}{2}} = 0.3$–3.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)
- $k_{\text{OH}} = 20.581 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{\frac{1}{2}} = 0.40$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^{6}$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:
- phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{\frac{1}{2}} = 4$ months to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)
- $k$(acid catalyzed) = 0.04 M$^{-1}$ h$^{-1}$, $k$(second order alkaline) = 59 M$^{-1}$ h$^{-1}$ in an aquatic environment (Wolfe et al. 1980a)
- $k$(base) = 7.4 M$^{-1}$ h$^{-1}$ at pH 7 and 25°C (Ellington et al. 1987)
- $t_{\frac{1}{2}} = 107$ yr at pH 7, $t_{\frac{1}{2}} = 1$ yr at pH 9 and 25°C (Howard et al. 1991; selected, Staples et al. 1997).

Biodegradation: the pseudo first-order degradation rate constant $k = 0.14 \text{ d}^{-1}$ corresponding to $t_{\frac{1}{2}} = 5$ d in a model ecosystem (Sanborn et al. 1975);
- degradation $t_{\frac{1}{2}} = 8$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
- rate constant $k = (1.57 \pm 0.17) \times 10^{2} \text{ min}^{-1}$ from retention times of reverse phase chromatography (estimated, Urushigawa & Yonezawa 1979);
- microbial degradation rate constant $k = 2 \times 10^{-4} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a)
significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate k < 0.5 d⁻¹ (Tabak et al. 1981; quoted, Mills et al. 1982); biodegradation rate constant k = 7.4 × 10⁻⁹ mL·cell⁻¹·d⁻¹ at 30°C in water (Scow 1982); aqueous aerobic t₁/₂ = 168–672 h, based on unacclimated and acclimated aqueous screening test data; aqueous anaerobic t₁/₂ = 4320–8760 h, based on acclimated anaerobic screening test data (Howard et al. 1991); rate constant k = 0.0014 h⁻¹ with t₁/₂ = 513.4 h for microbial degradation by anaerobic sludge (Wang et al. 2000) aerobic biodegradation in aquatic environments, first order k = 0.7 d⁻¹ with t₁/₂ = 1.0 d in river water (Peterson & Staples 2003) anaerobic biodegradation, first order rate k = 0.006–0.0336 d⁻¹ with t₁/₂ = 115–20.6 d in undiluted digester sludge of different DOP concn, batch incubation (Peterson & Staples 2003) Biotransformation: k = 3.1 × 10⁻¹⁰ mL·cell⁻¹·h⁻¹ for bacterial transformation in water (Wolfe et al. 1980a); microbial transformation k = (3.7 ± 0.6) × 10⁻¹³ L·organism⁻¹·h⁻¹ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

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

- k₂ = 3.69 × 10⁻⁵ d⁻¹ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)
- k₂ = 3.16 × 10⁻⁶ d⁻¹ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

- Air: t₁/₂ = 4.5–44.8 h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
- photodegradation t₁/₂ = 0.40 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10⁶ molecule cm⁻³ in air (Peterson & Staples 2003)
- Surface water: degradation t₁/₂ = 5 d in an aquatic model ecosystem (Sanborn et al. 1975); overall degradation t₁/₂ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
- biodegradation t₁/₂ = 1.0 d in aerobic aquatic environments (Peterson & Staples 2003)
- Ground water: t₁/₂ = 336–8760 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:
- Soil: degradation t₁/₂ = 8 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
- t₁/₂ = 10–50 d via volatilization subject to plant uptake from the soil (Ryan et al. 1988); degradation t₁/₂ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:
15.1.3.12 Di-isooctyl phthalate (DIOP)

Common Name: Di-isooctyl phthalate
Synonym: DIOP
Chemical Name:
CAS Registry No: 27554-26-3
Molecular Formula: C_{24}H_{38}O_{4}
Molecular Weight: 390.557
Melting Point (°C):
-4 (Fishbein & Albro 1972)
-46 (Staples et al. 1997)
Boiling Point (°C):
270 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
524.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.09 (shake flask-GC, Howard et al. 1985)
0.001; 0.00024, 0.00081 (recommended; calculated-QSAR, Staples et al. 1997)
2.49 × 10⁻³ (calculated-QSPR, Cousins & Mackay 2000)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.55 × 10⁻⁴ (dew-point and tensimeter methods, extrapolated from Clausius-Clapeyron eq., Werner 1952)
log (P/micron) = - 4829/(T/K) + 13.262; temp range 70–210°C, (exptl. data fitted to the Clausius-Clapeyron eq., Werner 1952)
7.4 × 10⁻⁴ (gas saturation method, Howard et al. 1985)
log (P/mmHg) = 24.8803 – 5.5821 × 10⁻³(T/K) – 1.547 × 10⁻²(T/K) + 6.5101 × 10⁻⁶(T/K)²; temp range 260–851 K (vapor pressure eq., Yaw et al. 1994)
1.55 × 10⁻⁴, 7.4 × 10⁻⁴, 4.53 × 10⁻⁵ (quoted, Staples et al. 1997)
7.5 × 10⁻⁴, 1.33 × 10⁻⁴, 2.67 × 10⁻⁸, 1.87 × 10⁻⁴ (recommended; calculated-QSAR, Staples 1997)
2.52 × 10⁻³ (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
3.95 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
8.0; 8.39 (recommended; calculated-QSAR, Staples et al. 1997)
7.73 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log K_{oa}:
10.53 (calculated-QSPR, Cousins & Mackay 2000)
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
  Volatilization:
  Photolysis:
  Oxidation: atmospheric photooxidation t_{1/2} ~ 0.3–3.0 d (Estimated, Staples et al. 1997).
  Hydrolysis: aqueous hydrolysis t_{1/2} ~ 157 yr (estimated, Staples et al. 1997).
  Biodegradation: primary biodegradation rate constant k = 0.082 d^{-1} and t_{1/2} = 8.82 d in an acclimated shake flask CO_{2} evolution test (Sugatt et al. 1984).
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
  Air: atmospheric photooxidation t_{1/2} ~ 0.3–3.0 d (estimated, Staples et al. 1997).
  Surface water: primary biodegradation rate constant k = 0.082 d^{-1} and t_{1/2} = 8.82 d in an acclimated shake flask CO_{2} evolution test (Sugatt et al. 1984);
  aqueous hydrolysis t_{1/2} ~ 157 yr (estimated, Staples et al. 1997).
  Groundwater:
  Sediment:
  Soil:
  Biota:
15.1.3.13  *bis-(2-Ethylhexyl) phthalate (DEHP)*

![Chemical structure of bis-(2-Ethylhexyl) phthalate](image)

Common Name: Di-(2-ethylhexyl) phthalate  
Synonym: DEHP, bis(2-ethylhexyl) phthalate, di-(2-ethylhexyl)orthophthalate, bis(2-ethylhexyl) phthalic acid ester, di-sec-octyl phthalate, 2-ethylhexyl phthalate, 1,2-benzenedicarboxylic acid bis(2-ethylhexyl) ester  
Chemical Name: bis(2-ethylhexyl) phthalate, di-sec-octyl phthalate, 2-ethylhexyl phthalate  
CAS Registry No: 117-81-7  
Molecular Formula: $C_{24}H_{38}O_4$, o-$C_6H_4(COOCH_2CH(C_2H_5)C_4H_9)2$  
Molecular Weight: 390.557

- Melting Point ($^{\circ}C$): -55.0 (Vershueren 1983; Lide 2003)
- Boiling Point ($^{\circ}C$): 384.0 (Dean 1985; Riddick et al. 1986; Lide 2003)
- Density (g/cm$^3$ at 20$^{\circ}C$): 0.9850 (Fishbein & Albro 1972), 0.9843 (Riddick et al. 1986)
- Molar Volume (cm$^3$/mol): 396.1 (20$^{\circ}C$, calculated-density, Stephenson & Malanowski 1987), 524.8 (calculated-Le Bas method at normal boiling point)
- Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol): 107.1, 105.9 (Small et al. 1948)
- Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
- Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
- Fugacity Ratio at 25$^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m$^3$ or mg/L at 25$^{\circ}C$):
- 100 (20$^{\circ}C$, Fishbein & Albro 1972)  
- 50.0 (from Monsanto Chemical Co. data sheets, Peakall 1975)  
- 0.60 (Branson 1978; Kenaga & Goring 1980)  
- 0.285 (shake flask-nephelometry on technical grade DEHP, Hollifield 1979)  
- 100 (quoted from Metcalf & Lu 1973, Hollifield 1979; Garten & Trabalka 1983)  
- 2.49 (Neely 1979; quoted, Neely & Blau 1985; Lyman 1985; Elzerman & Coates 1987)  
- 0.40 (shake flask-GC, Wolfe et al. 1979, 1980a, b)  
- 1.16 (solubility in 35 L instant ocean solution, Giam et al. 1980)  
- 0.047 (from OECD 1979/80, Klöppfer et al. 1982)  
- 0.041 (20$^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)  
- 0.34 ± 0.04 (shake flask-HPLC/UV, Howard et al. 1985)  
- < 100 (quoted, Riddick et al. 1986)  
- 0.27; 0.36 (centrifugation method, turbidity inflection method, DeFoe et al. 1990)  
- 9.8 × 10$^{-8}$ to 0.633 (lit. values, Sabljic et al. 1990)  
- 0.003 (recommended, Staples et al. 1997)  
- 0.0249 (calculated-QSPR, Cousins & Mackay 2000)  
- 0.017 (22$^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001)  
- 0.0019 (20$^{\circ}C$, shake flask-GC/MSD, Letinski et al. 2002)  
- 0.00285, 0.00024 (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
temperatures designated * are compiled at the end of this section):

1.45 × 10⁻⁵ (20°C, extrapolated, tensimeter, measured range 95–145°C, Hickman et al. 1937)
log (P/µmHg) = 15.116 – 5590/(T/K); temp range 95–145°C (Hickman et al. 1937)
1.93 × 10⁻³ (effusion method, extrapolated-Antoine eq., Small et al. 1948)
log (P/mmHg) = 12.12 – 5590/(T/K) (Antoine eq., quoted from Barclay & Butler 1938; Small et al. 1948)
log (P/mmHg) = 12.47 – 5757/(T/K); pressure range 5 × 10⁻² to 10⁻⁴ mmHg (effusion, data presented in graph
and Antoine eq., Small et al. 1948)

1.51 × 10⁻⁵ (20°C, extrapolated, tensimeter, measured range 99–148°C, Perry & Weber 1949)
log (P/µmHg) = 14.62 – 5440/(T/K); temp range 99–148°C (pendulum tensimeter method, Perry & Weber 1949)

8.26 × 10⁻⁶* (measured by dew-point and tensimeter methods, temp range 120–225°C, extrapolated from Antoine
eq., Werner 1952)
log (P/micron) = 12.639 – 3811/(201.2 + t/°C); temp range 120–225°C (Antoine eq., Dew-Point and Tensimeter
methods, data presented in graph, Werner 1952)

2.70 × 10⁻⁵ (20°C, calculated-Antoine eq., Weast 1972–73)
1.73 × 10⁻⁵ (submicron droplet evaporation, Chang & Davis 1976)
5.81 × 10⁻⁵ (36°C, submicron droplet evaporation, Davis & Ray 1977)

5.84 × 10⁻⁶ (17°C, submicron droplet evaporation, measured range 17–31°C, Ray et al. 1979)
log (P/mmHg) = 12.729 – 5822/(T/K); temp range 17–31°C (submicron droplet evaporation, Ray et al. 1979)
6.0 × 10⁻⁶*, 1.30 × 10⁻⁵ (20°C, effusion-vapor pressure balance, gas saturation method, OECD 1981)
log (P/mmHg) = 10.086 – 5010.357/(T/K); temp range 10–50°C (Antoine eq., gas saturation, OECD 1981)
log (P/mmHg) = 13.243 – 6035.017/(T/K); temp range 80–120°C (Antoine eq., effusion, OCED 1981)
5.50 × 10⁻⁶ (20°C, estimated-evaporation rate, Dobbs & Cull 1982)

7.01 × 10⁻⁸ (20°C, gas saturation, measured range 120–140°C, Potin-Gauthier et al. 1982)
log (P/mmHg) = 18.408 – 8112.265/(T/K); temp range 120–140°C (Potin-Gauthier et al. 1982)
0.00293, 1.87 × 10⁻⁶, 7.47 × 10⁻⁴ (estimation-structure based methods, Tucker et al. 1983)
8.6 ± 6.6) × 10⁻⁴ (gas saturation-HPLC/UV, Howard et al. 1985)
70, 700 (literature values, Riddick et al. 1986)
5.08 × 10⁻⁵ (extrapolation-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 11.8564 – 6416.2/(36.74 + T/K); temp range 373–660 K (Antoine eq., Stephenson & Malanowski
1987)

(1.20–2.40) × 10⁻⁵ (quoted from OECD interlaboratory studies, Hinckley et al. 1990)
1.90 × 10⁻⁵ (GC-RT correlation, Hinckley et al. 1990)
1.2 × 10⁻⁴* (40°C, OECD Vapour Pressure Curve Guideline 104, temp range 40–80°C, OECD 1993)
log (P/mmHg) = –0.7422 – 7.2012 × 10⁴/(T/K) + 9.9887·log(T/K) – 2.2697 × 10⁻²·(T/K) + 8.2181 × 10⁻⁶·(T/K)²;
temp range 350–886 K (vapor pressure eq., Yaw et al. 1994)

1.50 × 10⁻⁴* (40°C, Knudsen effusion with different orifice diameters and variable cell height, measured range
40–80°C, Goodman 1997)
log (P/Pa) = 14.90 – 5911/(T/K); temp range 40–80°C (Knudsen effusion, Goodman 1997)

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

0.0446 (calculated-P/C, Wolfe et al. 1980a)
1.1140 (calculated, Lyman et al. 1982)
0.0304 (20–25°C, calculated-P/C, Mabey et al. 1982)
0.0263, 3.14 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
0.0042 (estimated-P/C, Lyman 1985)
0.101 (estimated as per Hine & Mookerjee 1975, Lyman 1985)
0.0041 (calculated-P/C, Mackay 1985, Neely & Blau 1985)
0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
1.4940 (calculated-P/C, Meylan & Howard 1991)
1.1970 (estimated-bond contribution, Meylan & Howard 1991)
1.7324 (selected, Staples et al. 1997)
3.95 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log $K_{OW}$:

3.58 (Lu & Metcalf 1975)

4.20 (Mayer 1976)

5.30 (Hirzy et al. 1978)

8.73 (calculated, Wolfe et al. 1979)

5.11, 4.66–5.45 (shake flask method: mean, range, OECD 1981)

7.86 (HPLC-extrapolated from alkylbenzenes, Harnish et al. 1983)

5.03 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)

9.64 (quoted lit. calculated value, Leyder & Boulanger 1983)

7.94 (HPLC-RT correlation, Howard et al. 1985)

7.80, 8.90 (HPLC-RT correlation, TLC-RT, Klein et al. 1988)

7.453 ± 0.061 (slow-stirring-GC, DeBruijn et al. 1989)

5.22 (shake flask method, Brooke et al. 1990)

7.86, 9.68 (HPLC method, calculated, Brooke et al. 1990)

7.137 ± 0.153 (stir-flask method by BRE, Brooke et al. 1990)

7.453 ± 0.061 (stir-flask method by RITOX, Brooke et al. 1990)

7.88 (recommended, Sangster 1993)

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

10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

2.11 (fish, Metcalf et al. 1973)

5.03 (mosquito larvae, Metcalf et al. 1973)

4.13, 3.49, 3.72, 3.36, 2.36 (scud, midge larvae, waterflea, mayfly, sowbug, Sanders et al. 1973)

3.56, 2.54, 2.62, 2.76, 2.66 (scud, midge, waterflea, mayfly, fathead minnow, 14-d exposure, Mayer & Sanders 1973)

3.14 (fathead minnow, 28-d exposure, Mayer & Sanders 1973)

2.76 (fathead minnow, 56-d exposure, Mayer 1976)

2.93 (fathead minnow, Veith et al. 1979)

2.90, 2.15 (fathead minnow, Branson 1978)

2.06 (bluegill sunfish, Barrows et al. 1980)

–1.92 (adipose tissue of female Albino rats, Geyer et al. 1980)

3.95 (bacteria, calculated-$K_{OW}$, Wolfe et al. 1980a)

0.84–1.05, 1.01–1.22, 1.03–1.13 (oyster, shrimp, fish, Wofford et al. 1981)

1.04 (oyster, Wofford et al. 1981; quoted, Zaroogian et al. 1985)

2.93, 2.88 (fish: quoted, calculated-$K_{OW}$, Mackay 1982)

2.32 (Daphnia magna, Brown & Thompson 1982a)

3.37, 3.42, 3.40 (mussel Mytilus edulis, Brown & Thompson 1982b)

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

2.49, 2.11 (fish: flowing water, microcosm conditions, Graten & Trabalka 1983)

3.73, 3.57 (algae Chlorella, calculated-$K_{OW}$, Geyer et al. 1984)

2.80 (sheephead minnows, predicted-pharmacokinetic model, Karara & Hayton 1984)

2.66, 3.73, 3.48 (golden orfe, algae, activated sludge, Freitag et al. 1982)

1.60, 3.34, 3.48 (golden ide, algae, activated sludge, Freitag et al. 1983)

2.96, 2.87 (oyster, estimated values, Zaroogian et al. 1985)

2.96, 2.87 (sheephead minnows, estimated values, Zaroogian et al. 1985)

2.76 (quoted, Isnard & Lambert 1989)

0.204–1.71 (rainbow trout, BCF to decline as body wt. increased, Tarr et al. 1990)

2.94 (fish, highest fish BCF, Matthiessen et al. 1992)

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

4.0–5.0 (soil, calculated values, Kenaga 1980; Wolfe et al. 1980a)

4.756 (sediment-water, calculated-$K_{OW}$ and $S$, Wolfe et al. 1980a)

9.301 (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
Environmental Fate Rate Constants, k, and Half-Lives, t<sub>1/2</sub>:

Volatilezation: calculated evaporation rate k = 0.00052 cm/h corresponding to t<sub>1/2</sub> = 132600 h for a pond of 1 m deep (Branson 1978).

Photolysis: rate constant for direct photolysis k = 2 × 10<sup>-4</sup> h<sup>-1</sup> in natural water (Wolfe et al. 1980a);
- t<sub>1/2</sub> ~ 143 d in water is estimated to be 143 d (Wolfe et al. 1980a; quoted, Howard 1989);
- atmospheric t<sub>1/2</sub> = 3500–4800 h and aqueous t<sub>1/2</sub> = 3500–4800 h, based on measured rate of aqueous photolysis for DMP (Howard 1991).
- Aqueous photolysis k = 0.9 h<sup>-1</sup> and t<sub>1/2</sub> = 0.75 h (Jin et al. 1999, quoted, Peterson & Staples 2003)

Oxidation: the free radical oxidation rate constant k = 18 M·s<sup>-1</sup> (Wolfe et al. 1980b);
- photooxidation t<sub>1/2</sub> = 44–584 d in water, based on estimated rate constant for the reaction with hydroxyl radicals in water (Wolfe et al. 1980; quoted, Howard et al. 1991);
- rate constant k << 360 M<sup>-1</sup>·h<sup>-1</sup> for singlet oxygen and k = 7.2 M<sup>-1</sup>·h<sup>-1</sup> for peroxy radical (Mabey et al. 1982);
- photooxidation t<sub>1/2</sub> = 2.9–29 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
- predicted atmospheric photooxidation t<sub>1/2</sub> = 0.2–2.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).

k<sub>OH</sub> = 21.955 × 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> and t<sub>1/2</sub> = 0.38 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10<sup>6</sup> molecule cm<sup>-3</sup> in air (Peterson & Staples 2003)

Hydrolysis: second order alkaline hydrolysis rate constant k = 1.1 × 10<sup>-4</sup> M<sup>-1</sup>·s<sup>-1</sup> for pH 10–12 at 30°C in water (Wolfe et al. 1979, 1980b; quoted, Callahan et al. 1979);
- t<sub>1/2</sub> = 100 to 2000 yr for hydrolytic degradation alone in the eutrophic lake ecosystem at steady-state increase (Wolfe et al. 1980a);
- t<sub>1/2</sub>(calc) = 2000 yr at pH 7 in water (calculated per Radding et al. 1977; quoted, Callahan et al. 1979; Howard 1989; Howard et al. 1991);
- k(exptl.) = 9.5 × 10<sup>-7</sup> d<sup>-1</sup> at pH 7 and 25°C while estimated rate constant k = 1.46 × 10<sup>-6</sup> d<sup>-1</sup> at pH 7 and 30°C (Neely 1985);
- first-order hydrolysis t<sub>1/2</sub> = 2000 yr at pH 7, based on measured base catalyzed hydrolysis rate constant (Howard et al. 1991; selected, Staples et al. 1997).

Biodegradation: approximately calculated rate constant k = 0.091 d<sup>-1</sup> in pond water plus sediment incubated under aerobic conditions based on time for 50% degradation (Johnson & Lulve 1975; quoted, Klečka 1985); estimated biodegradation t<sub>1/2</sub> ~ 4–5 wk by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);
- degradation t<sub>1/2</sub> = 1.3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);
- rate constant k = 0.023 d<sup>-1</sup> in river water incubated under aerobic conditions (Klečka 1985);
- rate constant k(mineralization rate divided by initial substrate concn.) = 0.028 ± 0.013 d<sup>-1</sup> in lake water incubated under aerobic conditions (Subba-Rao et al. 1982; quoted, Klečka 1985);
- t<sub>1/2</sub> = 2.0–3.0 wk, based on river die-away test data (Hattori et al. 1975; Saeger & Tucker 1976; Wolfe et al. 1980; estimated, Howard 1989);
- t<sub>1/2</sub> = 0.8 d in activated sludge (Saeger & Tucker 1976; estimated, Howard 1989);
- microbial degradation rate constant k = 4.2 × 10<sup>-12</sup> mL·organism<sup>-1</sup>·s<sup>-1</sup> (Wolfe et al. 1980a); significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate k < 0.5 d<sup>-1</sup> (Tabak et al. 1981; quoted, Mills et al. 1982);

aqueous aerobic t<sub>1/2</sub> = 120–550 h, based on grab sample die-away test data (Schouten et al. 1979 and Johnson & Lulve 1975; estimated, Howard et al. 1991);
die-away test data (Howard et al. 1991) and anaerobic aqueous screening studies (Horowitz et al. 1982 and Shelton et al. 1984; estimated, Howard et al. 1991);
mean rate constant $k = 0.136 \text{ d}^{-1}$ corresponding to $t_{1/2} = 5.25 \text{ d}$ in shake flask biodegradation experiment (Sugatt et al. 1984);
more than 90% of initial 3.3 mg/L will be degraded in activated sludge systems in 2–5 d (O’Grady et al. 1985);
greater than 50% loss in microbial degradation in less than 20 d under aerobic conditions, very low under anaerobic conditions in garden soil (Shanker et al. 1985);
readily metabolized in uninoculated Erie slit loam with the absence of nonaqueous-phase liquids (NAPLs) for about 20 d (Efroymson & Alexander 1994)
biphasic microbial mineralization kinetics: $k = 0.0044 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ at 5°C, $k = 0.0081 \text{ d}^{-1}$ with $t_{1/2} = 86 \text{ d}$ at 10°C, and $k = 0.0134 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ at 20°C in agriculture soil for phase I; and $t_{1/2} = 224 \text{ d}$ at 5°C, $t_{1/2} = 187 \text{ d}$ at 10°C and $t_{1/2} = 73 \text{ d}$ at 20°C in agriculture soil for phase II. Rate $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ at 5°C, $k = 0.0055 \text{ d}^{-1}$ with $t_{1/2} = 125 \text{ d}$ at 10°C, and $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ at 20°C in sludge-amended soil for phase I and $t_{1/2} \geq 365 \text{ d}$ at 5°C, $t_{1/2} = 337 \text{ d}$ at 10°C and $t_{1/2} = 150 \text{ d}$ at 20°C in sludge-amended soil for phase II kinetics in laboratory microcosms. At 20°C, aerobic mineralization rate $k = 0.0182 \text{ d}^{-1}$ with $t_{1/2} = 37 \text{ d}$ for phase I, $t_{1/2} = 51 \text{ d}$ for phase II in well-mixed sludge, $k = 0.0058 \text{ d}^{-1}$ with $t_{1/2} = 120 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in aggregate sludge, aerobic $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ for phase I, $t_{1/2} = 150 \text{ d}$ for phase II and anaerobic $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in sludge-amended soil (Madsen et al. 1999).
aerobic biodegradation in aquatic environments, first order $k = 0.023 \text{ d}^{-1}$ with $t_{1/2} = 30 \text{ d}$ in unstirred river water, $k = 0.2 \text{ d}^{-1}$ with $t_{1/2} = 3.5 \text{ d}$ in shaken river water, $k = 1.73 \text{ d}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ field data, estuarine sediment (Peterson & Staples 2003)
aerobic soil degradation, pseudo-first-order $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ in loam; $k = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 69.3 \text{ d}$ in sand; $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in outdoor lysimeter, loam; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in outdoor lysimeter, sand; $k = 0.12 \text{ d}^{-1}$ with $t_{1/2} = 5.6 \text{ d}$ in garden soil; $k = 0.040 \text{ d}^{-1}$ with $t_{1/2} = 17.3 \text{ d}$ in soil with 2% OC-organic carbon; $k = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 36.5 \text{ d}$ in soil with 3.3% OC; $k = 0.015 \text{ d}^{-1}$ with $t_{1/2} = 46.2 \text{ d}$ in soil with 1.6% OC and $k = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 58 \text{ d}$ in sludge amended loam. For anaerobic degradation, first order rate $k > 0.3 \text{ d}^{-1}$ with $t_{1/2} < 2.3 \text{ d}$ in undiluted digester sludge, batch incubation; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in flood soil; $k = 0.69 \text{ d}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ field data, sediment (Peterson & Staples 2003)
Biotransformation: $k = 4.2 \times 10^{-12} \text{ mL.cell}^{-1}.\text{h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982); microbial transformation $k = (4.2 \pm 0.7) \times 10^{-15} \text{ L.organism}^{-1}.\text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:
$\text{t}_{1/2} = 7 \text{ d}$ for elimination of DEHP from fathead minnows (Mayer & Sanders 1973);
fish elimination $\text{t}_{1/2} = 6.2$ to 18.3 d with a mean value of 12.2 d after 56 d exposure period (fathead minnows, Mayer 1976);
$k_1 = 76 \text{ mL g}^{-1}.\text{h}^{-1}$ (fish, Branson 1978);
depuration $\text{t}_{1/2} = 72 \text{ h}$ (tissues of bluegill sunfish, Barrows et al. 1980).
$k_2 = 3.69 \times 10^{-3} \text{ d}^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)
$k_2 = 3.16 \times 10^{-6} \text{ d}^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)
Half-Lives in the Environment:
Air: $\text{t}_{1/2} = \text{half-life of 2.9–29 h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
Photodegradation $\text{t}_{1/2} = 0.38 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)
Surface water: biodegradation $\text{t}_{1/2} \sim 4$ to 5 wk in river water by naturally occurring, mixed microbial populations (Saeger & Tucker 1976);
$\text{t}_{1/2} = 5 \text{ d}$ in a model ecosystem (Verschueren 1983);
$\text{t}_{1/2} = 5.25 \text{ d}$ in an acclimated shake flask CO2 evolution biodegradation experiment (Sugatt et al. 1984)
$\text{t}_{1/2} = 120-550 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biodegradation $t_{1/2} = 0.3$–$30\text{ d}$ in estuarine river water with sediment and river water (Peterson & Staples 2003).

Ground water: $t_{1/2} = 240$–$9336\text{ h}$, based on unacclimated aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

- degradation $t_{1/2} = 39\text{ d}$ for initial phase, $t_{1/2} = 51\text{ d}$ for the late phase in sludge-amended quartz; $t_{1/2} = 58\text{ d}$ for initial phase and $t_{1/2} = 147\text{ d}$ for sludge-amended soil, $t_{1/2} = 58\text{ d}$ for initial phases and $t_{1/2} = 84\text{ d}$ in sludge slurry; $t_{1/2} = 9\text{ d}$ for initial phases, $t_{1/2} = 35\text{ d}$ for late phase in sludge-amended soil + strain SDE-2 (Roslev et al. 1998)
- overall $t_{1/2} = 120$–$550\text{ h}$, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

degradation by microorganism in biometer systems, $t_{1/2} = 66\text{ d}$ in silty sand standard metabolism experiments, $t_{1/2} = 102\text{ d}$ corrected standard conditions, $t_{1/2} = 170\text{ d}$ in simulated outdoor conditions; $t_{1/2} = 20\text{ d}$ in silty loam standard conditions, $t_{1/2} = 30\text{ d}$ corrected standard conditions, $t_{1/2} = 31\text{ d}$ in simulated outdoor conditions at constant soil moisture and $20^\circ\text{C}$; degradation by microorganism in outdoor experiments in small lysimeter systems: $t_{1/2} = 54\text{ d}$ outdoor fallow and $t_{1/2} = 200\text{ d}$ outdoor barley in silty sand, and $t_{1/2} = 21\text{ d}$ outdoor fallow, $t_{1/2} = 14\text{ d}$ outdoor barley in silty loam (Rüdel et al. 1993)

microbial mineralization $t_{1/2} = 158$, $86$ and $52\text{ d}$ at $5$, $10$, and $20^\circ\text{C}$, respectively, in soil; $t_{1/2} = 301$, $125$ and $55\text{ d}$ at $5$, $10$ and $20^\circ\text{C}$ in sludge-amended soil in phase I degradation kinetics; $t_{1/2} = 224$, $187$ and $73\text{ d}$ at $5$, $10$, and $20^\circ\text{C}$, respectively, in soil; $t_{1/2} = 365$, $337$ and $150\text{ d}$ at $5$, $10$ and $20^\circ\text{C}$ in sludge-amended soil in phase II degradation kinetics. At $20^\circ\text{C}$, $t_{1/2}$ varies between $77$–$89\text{ d}$ and $100$–$127\text{ d}$ for phase I and II, respectively, in sludge-amended soil with different initial DEHP concns. Aerobic $t_{1/2} = 37\text{ d}$ and $51\text{ d}$ for phase I and II in well mixed sludge, $t_{1/2} = 120\text{ d}$ and $> 365\text{ d}$ for phase I and II in aggregate sludge, $t_{1/2} = 55\text{ d}$ and $150\text{ d}$ for phase I and II in sludge-amended soil; anaerobic $t_{1/2} = 301\text{ d}$ and $> 365\text{ d}$ for phase I and II in sludge-amended soil (laboratory microcosms, Madsen et al. 1999)

biodegradation in aerobic soil: $t_{1/2} = 2.0$ – $69.3\text{ d}$ in various sand, loam, soils with different organic carbon content and sludge amended loam in laboratory and outdoor experiments (Peterson & Staples 2003)

Biota: elimination and degradation $t_{1/2} < 4\text{ d}$ after $7\text{ d}$ for water fleas $Daphnia magna$ and $t_{1/2} = 7\text{ d}$ for fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2} = 12.2\text{ d}$ (fathead minnows $Pimephales promelas$, Mayer 1976);

depuration $t_{1/2} = 3\text{ d}$ (in tissues of bluegill sunfish continuously for $42\text{-d}$ exposure, Barrows et al. 1980)

depuration $t_{1/2} = 38\text{ d}$ from sheephead minnow (Karara & Hayton 1984).

**TABLE 15.1.3.13.1**

Reported vapor pressures of bis(2-ethylhexyl) phthalate (DEHP) at various temperatures and the coefficients for the vapor pressure equations

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

OECD 1981

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OECD 1993

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Knudsen effusion

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Goodman 1997

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**FIGURE 15.1.3.13.1** Logarithm of vapor pressure versus reciprocal temperature for bis(2-ethylhexyl) phthalate.
15.1.3.14 Di(hexyl,octyl,decyl) phthalate

Common Name: Di(hexyl,octyl,decyl) phthalate
Synonym: 610P
Chemical Name:
CAS Registry No: 25724-58-7, 68515-51-5
Molecular Formula: C_{25}H_{40}O_{4}
Molecular Weight: 404.583

Melting Point (°C):
-4 (Staples et al. 1997)

Boiling Point (°C):

Density (g/cm³ at 20°C):

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
0.9 ± 0.5 (shake flask, Howard et al. 1985)
0.05; 0.0004 (recommended; calculated-QSAR, Staples et al. 1997)
8.76 × 10⁻¹ (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
6.5 × 10⁻⁴ (gas saturation, Howard et al. 1985)
6.5 × 10⁻⁴; 4.53 × 10⁻⁵, 6.5 × 10⁻² (recommended; calculated-QSAR, Staples et al. 1997)
1.31 × 10⁻⁵ (calculated-QSPR, Cousins & Mackay 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C):
6.05 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
5.9–8.61 (HPLC-RT correlation, Howard et al. 1985; quoted, Staples et al. 1997)
7.25; 8.54 (recommended; calculated-QSAR, Staples et al. 1997)
8.17 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
10.78 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: atmospheric photooxidation t_{1/2} ~ 0.2–4.0 d (estimated, Staples et al. 1997).
Hydrolysis:
Biodegradation: primary biodegradation with a rate constant k = 0.131 d⁻¹ and t_{1/2} = 5.30 d in an acclimated shake flask CO₂ evolution test (Sugatt et al. 1984).
Biotransformation:
Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:
Half-Lives in the Environment:

Air: atmospheric photooxidation \( t_{1/2} \approx 0.2-4.0 \text{ d} \) (estimated, Staples et al. 1997).

Surface water: primary biodegradation with a rate constant \( k = 0.131 \text{ d}^{-1} \) and \( t_{1/2} = 5.30 \text{ d} \) in an acclimated shake flask CO\(_2\) evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:
15.1.3.15 Diisononyl phthalate (DINP)

Common Name: Diisononyl phthalate
Synonym: DINP
Chemical Name:
CAS Registry No: 28553-12-0, 68515-48-0
Molecular Formula: C_{26}H_{42}O_{4}
Molecular Weight: 418.609
Melting Point (°C):
  -48 (Staples et al. 1997)
Boiling Point (°C):
  413 (Fishbein & Albro 1972)
Density (g/cm³ at 20°C):
  0.995 (Fishbein & Albro 1972)
Molar Volume (cm³/mol):
  569.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  0.20 ± 0.1 (shake flask-GC, Howard et al. 1985)
  0.20, 0.0006 (quoted, Staples et al. 1997)
  < 0.001; 7.8 × 10⁻⁵, 2.3 × 10⁻³ (recommended; calculated-QSAR, Staples et al. 1997)
  3.08 × 10⁻⁴ (calculated-QSPR, Cousins & Mackay 2000)
  6.1 × 10⁻⁴ (20°C, shake flask/slow stirring-GC/MS, Letinski et al. 2002)
Vapor Pressure (Pa at 25°C):
  7.2 × 10⁻⁵ (gas saturation method, Howard et al. 1985)
  6.67 × 10⁻⁵; 1.33 × 10⁻⁸, 3.07 × 10⁻⁵ (recommended; calculated-QSAR, Staples et al. 1997)
  6.81 × 10⁻⁶ (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
  9.26 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
  > 8.0; 9.0, 9.4 (recommended; calculated-QSAR, Staples et al. 1997)
  8.60 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log K_{oa}:
  11.03 (calculated-QSPR, Cousins & Mackay 2000)
Bioconcentration Factor, log BCF:
  3.27 (Arca zebra, Solbakken et al. 1985)
Sorption Partition Coefficient, log \( K_{OC} \): 

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

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation \( t_\frac{1}{2} \sim 0.2\text{–}2.0 \text{ d} \) (estimated, Staples et al. 1997).

\[ k_{OH} = 23.408 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } t_\frac{1}{2} = 0.35 \text{ d} \text{ based on a global, seasonal and diurnal average OH radical concn of } 1 \times 10^6 \text{ molecule cm}^{-3} \text{ in air} \] (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant \( k = 0.131 \text{ d}^{-1} \) and \( t_\frac{1}{2} = 5.31 \text{ d} \) in an acclimated shake flask \( \text{CO}_2 \) evolution test (Sugatt et al. 1984).

Biotransformation:

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

\[ k_1 = 848 \text{ mL} \cdot \text{g} \cdot \text{d}^{-1} \text{ (Arca zebra, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)} \]
\[ k_2 = 0.46 \text{ d}^{-1} \text{ (Arca zebra, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)} \]
\[ k_2 = 0.02 \text{ d}^{-1} \text{ (Diplora strigosa, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)} \]

Half-Lives in the Environment:

Air: atmospheric photooxidation \( t_\frac{1}{2} \sim 0.2\text{–}2.0 \text{ d} \) (estimated, Staples et al. 1997).

Photodegradation \( t_\frac{1}{2} = 0.35 \text{ h} \text{ based on a global, seasonal and diurnal average OH radical concn of } 1 \times 10^6 \text{ molecule cm}^{-3} \text{ in air} \) (Peterson & Staples 2003)

Surface water: primary biodegradation with a rate constant \( k = 0.131 \text{ d}^{-1} \) and \( t_\frac{1}{2} = 5.31 \text{ d} \) in an acclimated shake flask \( \text{CO}_2 \) evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:
15.1.3.16 Di-isodecyl phthalate (DIDP)

Common Name: Di-isodecyl phthalate
Synonym: DIDP
Chemical Name: di-diisodecyl phthalate
CAS Registry No: 26761-40-0, 68515-49-1
Molecular Formula: C_{28}H_{46}O_{4}
Molecular Weight: 446.663
Melting Point (°C):
-48 (Stephenson & Malanowski 1987)
-46 (Staples et al. 1997)
-50 (Lide 2003)
Boiling Point (°C):
450 (Stephenson & Malanowski 1987)
Density (g/cm³ at 20°C):
464.8 (Stephenson & Malanowski 1987)
613.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
< 50 (quoted from Monsanto Chemical Co. data sheets, Peakall 1975)
1.19 ± 0.19 (shake flask-GC, Howard et al. 1985)
0.28 (shake flask-nephelometry, Hollifield 1979)
0.19, 0.28, < 0.00013 (quoted, Staples et al. 1997)
< 0.001; 2.2 × 10⁻⁴, 7.4 × 10⁻⁴ (recommended, calculated-QSAR, Staples et al. 1997)
3.81 × 10⁻³ (calculated-QSPR, Cousins & Mackay 2000)
1.7 × 10⁻⁴ (20°C, shake flask/slow stirring-GC/MS, Letinski et al. 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\[
\log (P_L/kPa) = 14.0158 - 10984/(242.24 + T/K), \text{ temp range: 371–496 K, (Antoine eq., Stephenson & Malanowski 1987)}
\]
\[
\log (P_{/mmHg}) = 81.7895 - 7.4225 \times 10^3/(T/K) - 26.916-\log (T/K) + 1.1502 \times 10^{-2}-(T/K) - 4.353 \times 10^{-14}-(T/K)^2; \text{ temp range 233–723 K (vapor pressure eq., Yaw et al. 1994)}
\]
6.67 × 10⁻³, 7.47 × 10⁻⁴ (quoted, Staples et al. 1997)
6.67 × 10⁻³; 6.67 × 10⁻⁶, 4.93 × 10⁻⁴, 1.33 × 10⁻⁸ (recommended, calculated-QSAR, Staples et al. 1997)
1.84 × 10⁻⁶ (calculated-QSPR, Cousins & Mackay 2000)
Henry’s Law Constant (Pa·m³/mol at 25°C):
21.6 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
7.70 (estimated, Williams et al. 1995)
> 8.0; 10.0, 1.0.3 (recommended; calculated-QSAR, Staples et al. 1997)
9.46 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log $K_{OA}$:
11.52 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:
1.95–2.1, 2.06 ($Daphnia magna$, 20°C, range, mean, Brown & Thompson 1982a)
3.48, 3.60; 3.54 ($Mytilus edulis$, 15°C, exposure concn: 4.4, 4.17 µg/L; mean value, Brown & Thompson 1982b)

Sorption Partition Coefficient, log $K_{OC}$:
5.04, 5.78, 5.16 (soil/sediment, exptl. data, Williams et al. 1995)
5.46, 7.60 (soil/sediment: mean value, calculated-KOW, Williams et al. 1995)

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

Volatilization:

Photolysis:
Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2$–2.0 d (estimated, Staples et al. 1997).

$K_{OH} = 26.217 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003).

Hydrolysis:
Biodegradation: degradation $t_{1/2} = 4.0$ d by microorganisms ($Pseudomonas acidovorans$ 256–1) from soil or waste water at 30°C (Kurane et al. 1977);
primary biodegradation with a rate constant $k = 0.088$ d$^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

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

$k_1 = 795, 539$ mL·g·d$^{-1}$ ($Mytilus edulis$, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

$k_2 = 0.20, 0.18$ d$^{-1}$ ($Mytilus edulis$, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

Half-Lives in the Environment:
Air: atmospheric photooxidation $t_{1/2} \sim 0.2$–2.0 d (estimated, Staples et al. 1997).
photodegradation $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003).

Surface water: primary biodegradation with a rate constant $k = 0.088$ d$^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

Groundwater:
Sediment:
Soil: degradation $t_{1/2} = 4.0$ d by microorganisms ($Pseudomonas acidovorans$ 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota: depuration $t_{1/2} = 3.5$ and 3.8 d DIDP concn at 5 and 50 µgL$^{-1}$ for $Mytilus edulis$ at 15°C (Brown & Thompson 1982b).
15.1.3.17 Diundecyl phthalate (DUP)

Common Name: Diundecyl phthalate
Synonym: DUP
Chemical Name: Diundecyl phthalate
CAS Registry No: 3648-20-2
Molecular Formula: C_{30}H_{50}O_{4}
Molecular Weight: 474.716
Melting Point (°C):
-9 (Staples et al. 1997)
35.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
0.96 (Staples et al. 1997)
Molar Volume (cm³/mol):
658.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.789 (mp at 35.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.11 ± 0.28 (shake flask, Howard et al. 1985)
< 0.001; 1.6 × 10⁻⁷, 4.2 × 10⁻⁷ (recommended; calculated-QSAR, Staples et al. 1997)
2.14 × 10⁻⁸ (calculated-UNIFAC, Thomsen et al. 1999)
4.41 × 10⁻⁶ (calculated-QSPR, Cousins & Mackay 2000)
Vapor Pressure (Pa at 25°C):
6.67 × 10⁻⁵, 7.07 × 10⁻⁵ (quoted, Staples et al. 1997)
6.67 × 10⁻⁵; 1.33 × 10⁻⁶, 1.6 × 10⁻⁷ (recommended; calculated-QSAR, Staples et al. 1997)
4.97 × 10⁻⁷ (calculated-QSPR, Cousins & Mackay 2000)
Henry's Law Constant (Pa·m³/mol at 25°C):
50.5 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log K_{ow}:
> 8.0; 11.2, 11.5 (recommended; calculated-QSAR, Staples et al. 1997)
10.54 (calculated-UNIFAC, Thomsen et al. 1999)
10.33 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Air Partition Coefficient, log K_{oa}:
12.02 (calculated-QSPR, Cousins & Mackay 2000)
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization:
Photolysis:
Oxidation: atmospheric photooxidation $t_{\text{oh}} \sim 0.2$–2.0 d (estimated, Staples et al. 1997).

\[ k_{\text{OH}} = 31.847 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

and $t_{\text{oh}} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation rate constant $k = 0.115$ d$^{-1}$ and $t_{\text{bi}} = 6.17$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

aerobic biodegradation in aquatic environments, first order $k = 0.03$ d$^{-1}$ with $t_{\text{bi}} = 23$ d in unstirred river water (Peterson & Staples 2003)

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{\text{oh}} \sim 0.2$–2.0 d (estimated, Staples et al. 1997)

Photodegradation $t_{\text{oh}} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant $k = 0.115$ d$^{-1}$ and $t_{\text{bi}} = 6.17$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

biodegradation $t_{\text{bi}} = 23$ d in aerobic aquatic environments (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil:

Biota:
15.1.3.18 Ditridecyl phthalate (DTDP)

Common Name: Ditridecyl phthalate

Synonym: DTDP

Chemical Name:

CAS Registry No: 119-06-2, 68515-47-9
Molecular Formula: C_{34}H_{58}O_{4}
Molecular Weight: 530.823

Melting Point (°C): 
-37 (Staples et al. 1997)

Boiling Point (°C): 

Density (g/cm³ at 20°C): 
0.953 (Staples et al. 1997)

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

0.34 (shake flask-nephelometry, Hollifield 1979)
< 0.30 (shake flask, Howard et al. 1985; quoted, Adams et al. 1995)
0.34, < 0.30 (quoted, Staples et al. 1997)
< 0.001; 1.5 × 10⁻⁹, 4.2 × 10⁻⁹ (recommended, calculated-QSAR, Staples et al. 1997)
4.07 × 10⁻¹⁰ (calculated-QIFAC, Thomsen et al. 1999)
7.0 × 10⁻⁸ (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
< 6.67 × 10⁻⁵ (quoted, Staples et al. 1997)
< 6.67 × 10⁻⁵; 1.33 × 10⁻⁵, 3.33 × 10⁻⁵ (recommended; calculated-QSAR, Staples et al. 1997)
3.63 × 10⁻⁸ (calculated-QSPR, Cousins & Mackay 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C):
275 (calculated-QSPR, Cousins & Mackay 2000)

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

8.40 (estimated, Williams et al. 1995)
> 8.0; 13.1, 13.4 (recommended; calculated-QSAR, Staples et al. 1997)
12.28 (calculated-UNIFAC, Thomsen et al. 1999)
12.06 (calculated-QSPR, Cousins & Mackay 2000)

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

13.01 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.08 (soil/sediment, Williams et al. 1995; quoted, Staples et al. 1997)
Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation t_1/2 ~ 0.2–2.0 d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation t_1/2 = 10.5 d by microorganisms \( Pseudomonas acidovorans \) 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation rate constant k = 0.029 d \(^{-1}\) and t_1/2 = 27.6 d in an acclimated shake flask CO\(_2\) evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k\(_1\)) and Elimination (k\(_2\)) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation t_1/2 ~ 0.2–2.0 d (estimated, Staples et al. 1997).

Surface water: primary biodegradation rate constant k = 0.029 d \(^{-1}\) and t_1/2 = 27.6 d in an acclimated shake flask CO\(_2\) evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation t_1/2 = 10.5 d by microorganisms \( Pseudomonas acidovorans \) 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:
15.1.3.19 Butyl benzyl phthalate (BBP)

Common Name: Butyl benzyl phthalate
Synonym: BBP, benzyl butyl phthalate
Chemical Name: butyl benzyl phthalate, benzyl butyl phthalate
CAS Registry No: 85-68-7
Molecular Formula: C_{19}H_{20}O_{4}, C_6H_5COOCH_2C_6H_4COOC_4H_9
Molecular Weight: 312.360

Melting Point (°C):
-35.0 (Callahan et al. 1979; Mabey et al. 1982; Howard 1989)

Boiling Point (°C):
370.0 (Verschueren 1983; Howard 1989; Lide 2003)

Density (g/cm³ at 20°C):
1.111 (Staples et al. 1997)

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

Enthalpy of Fusion, ΔH_fus (kJ/mol):

Entropy of Fusion, ΔS_fus (J/mol K):

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

Water Solubility (g/m³ or mg/L at 25°C):
- 2.90 (Hirzy et al. 1978)
- 0.71 (shake flask-nephelometry, practical grade, Hollifield 1979)
- 2.9 ± 1.2 (shake flask-GC, Gledhill et al. 1980)
- 40.2 (shake flask-LSC, Veith et al. 1980)
- 2.82 (20°C, shake flask-UV, Leyder & Boulanger 1983)
- 2.90 ± 1.2 (Verschueren 1983)
- 2.69 ± 0.15 (shake flask-HPLC/UV, Howard et al. 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
- 0.00115 (20°C, Gledhill et al. 1980)
- 0.00799 (calculated using Truton’s rule, Mabey et al. 1982)
- 0.00115 (Petrasek et al. 1983)
- 0.00115 (20°C, Verschueren 1983)
- log (P_t/kPa) = 9.1472 – 4647.5/(T/K), temp range: 416–516 K, (Antoine eq., Stephenson & Malanowski 1987)
- 0.0011, 0.00133 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
- 0.0067 (recommended, Staples et al. 1997)
- 0.0249 (calculated-QSPR, Cousins & Mackay 2000)

Henry’s Law Constant (Pa·m³/mol at 25°C):
- 0.132 (calculated-P/C, Wolfe et al. 1980a)
- 0.132 (calculated, Lyman et al. 1982)
- 0.841 (calculated-P/C, Mabey et al. 1982)
- 0.104 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 0.077 (selected, Staples et al. 1997)
- 0.205 (calculated-QSPR, Cousins & Mackay 2000)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 4.80 (Hirzy et al. 1978)
- 5.80 (calculated as per Leo et al. 1971)
- 4.77 (shake flask-GC analysis of both phases, Gledhill et al. 1980)
- 4.05 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
- 4.75 (RPHPLC-RT correlation, Veith et al. 1980)
- 3.97 (HPLC-$k'$ correlation, McDuffie 1981)
- 4.11, 3.23–4.45 (shake flask method: mean, range, OECD 1981)
- 4.91 (20°C, shake flask-UV, Leyder & Boulanger 1983)
- 4.78 (Verschueren 1983)
- 3.57 (HPLC-RT correlation, Howard et al. 1985)
- 4.91 (calculated, Hansch & Leo 1985)
- 4.87 (calculated-CLOGP, Müller & Klein 1992)
- 4.59 (recommended, Staples et al. 1997)
- 4.70 (calculated-QSPR, Cousins & Mackay 2000)

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

- 8.78 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log $BCF$:

- 2.74–3.34 (calculated-$K_{OW}$, Veith et al. 1979, 1980)
- 2.82 (bluegill sunfish, Barrows et al. 1980)
- 2.71 (calculated-$K_{OW}$, Gledhill et al. 1980)
- 2.82 (bluegill sunfish, quoted, Gledhill et al. 1980)
- 2.19–2.95 (fathead minnows, quoted, Gledhill et al. 1980)
- 2.89 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 3.90 (calculated-$K_{OW}$, Wolfe et al. 1980a)
- 4.67 (microorganisms-water, calculated-$K_{OW}$, Mabey et al. 1982)
- 3.57 (sediment, calculated-$K_{OW}$, Pavlou & Weston 1983, 1984)
- 2.89 (quoted, Isnard & Lambert 1988; quoted, Banerjee & Baughman 1991)
- 2.72 (calculated-$K_{OW}$ and $S_{octanol}$, Banerjee & Baughman 1991)

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

- 1.83–2.54 (soil, batch equilibration-GC, Gledhill et al. 1980)
- 3.95 (soil/sediment, Gledhill et al. 1980)
- 3.81 (calculated-$K_{OW}$, Wolfe et al. 1980a)
- 5.23 (sediment-water, calculated-$K_{OW}$, Mabey et al. 1982)
- 4.23 (Broome County soil in New York, Russell & McDuffie)
- 4.23, 3.97 (soil, quoted, calculated-MCI and fragment contribution, Meylan et al. 1992)
- 2.60 (activated carbon, calculated-MCI, Blum et al. 1994)
- 3.21 (quoted or calculated-QSAR MCI $\chi^1$, Sabljic et al. 1995)
- 5.00 (suspended solids, calculated-$K_q$ assuming a 0.1 org. carbon fraction, Staples et al. 1997)
- 3.21, 3.88; 3.11, 3.07, 3.21, 3.32, 3.15 (soil: quoted lit., calculated-$K_{OW}$; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization:

- Photolysis: direct photolysis (near surface) rate constant $k = 2 \times 10^{-4}$ h$^{-1}$ in natural water (Wolfe et al 1980a); photodegradation $t_{1/2} > 100$ d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989).
- Oxidation: the free radical oxidation rate constant $k = 18$ M$^{-1}$s$^{-1}$ for reaction with peroxy radical (Wolfe et al. 1980a);
  rate constant $k << 360$ M$^{-1}$h$^{-1}$ for singlet oxygen and $k = 280$ M$^{-1}$h$^{-1}$ for peroxy radical (Mabey et al. 1982);
  photooxidation $t_{1/2} = 6–60$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
predicted atmospheric photooxidation $t_{\frac{1}{2}} = 0.5–5.0$ d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).

$k_{OH} = 11.049 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $t_{\frac{1}{2}} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003).

Hydrolysis: the alkaline hydrolysis rate constant $k \sim 38$ M$^{-1}$h$^{-1}$; hydrolytic $t_{\frac{1}{2}} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

chemical degradation (hydrolysis) $t_{\frac{1}{2}} > 100$ d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989; selected, Staples et al. 1997).

Biodegradation: degradation $t_{\frac{1}{2}} \sim 2$ d in river water and $t_{\frac{1}{2}} = 2$ h in activated sludge (Saeger & Tucker 1976) degradation $t_{\frac{1}{2}} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977) microbial degradation rate constant $k = 2.9 \times 10^{-8}$ mL-organism$^{-1}$·s$^{-1}$ (Wolfe et al. 1981a);

0–24% mineralization in $> 8$ wk in municipal digested sludge (Horowitz et al. 1982);

primary degradation accounted for $> 95\%$ loss in 7 d with an initial concentration of 1.0 mg/L in a lake water microcosm with $t_{\frac{1}{2}} = < 4$ d and 100% primary degradation was observed after 9 d while $t_{\frac{1}{2}} = 2.0$ d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989);

significant degradation with rapid adaptation within 7 d in an aerobic environment with $k > 0.5$ d$^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

degradation rate constant $k = 0.043$ d$^{-1}$ corresponding to $t_{\frac{1}{2}} = 19.4$ d in a shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% degraded within 40 d in digested sludge (Shelton et al. 1984);

99% degraded in activated sludge systems in 48 h (O’Grady et al. 1985);

anaerobic digestion of sludge with first-order rate constant $k = 6.5 \times 10^{-3}$ h$^{-1}$ and $t_{\frac{1}{2}} = 107$ h (Ziougu et al. 1989);

aqueous aerobic $t_{\frac{1}{2}} = 24–168$ h, based on unacclimated river die-away test and aqueous anaerobic $t_{\frac{1}{2}} = 672–4320$ h, based on unacclimated anaerobic screening test data (Howard et al. 1991)

Aerobic biodegradation in aquatic environments, first order $k = 0.46$ d$^{-1}$ with $t_{\frac{1}{2}} = 1.5$ d in unstrirred river water, $k = 0.50$ d$^{-1}$ with $t_{\frac{1}{2}} = 1.4$ d in microcosm, lake, $k = 0.35$ d$^{-1}$ with $t_{\frac{1}{2}} = 2.0$ d in river water, $k = 0.14$ d$^{-1}$ with $t_{\frac{1}{2}} = 5.0$ d in microcosm, un-impacted, $k > 0.023$ d$^{-1}$ with $t_{\frac{1}{2}} < 3.0$ d in microcosm, Illinois river, and $k = 2.2$ d$^{-1}$ with $t_{\frac{1}{2}} = 0.32$ d in shake river water (Peterson & Staples 2003)

Anaerobic biodegradation $k = 0.056$ d$^{-1}$ with $t_{\frac{1}{2}} = 12.4$ d in undiluted sludge, batch incubation, $k = 0.19$ d$^{-1}$ with $t_{\frac{1}{2}} = 3.7$ d in undiluted sludge, $k = 0.096$ d$^{-1}$ with $t_{\frac{1}{2}} = 7.2$ d in 10% dilute sludge; $k = 0.076$ d$^{-1}$ with $t_{\frac{1}{2}} = 9.1$ d in 10% freshwater sediment and $k = 0.051$ d$^{-1}$ with $t_{\frac{1}{2}} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

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

microbial transformation $k = (3.1 \pm 0.8) \times 10^{-11}$ L-organism$^{-1}$·h$^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

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

depuration $t_{\frac{1}{2}} < 24$ and $> 48$ h from tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 0.0464$ d$^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.00397$ d$^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{\frac{1}{2}} = 1.5$ d in the atmosphere (GEMS 1984; quoted, Howard 1989);

t$\frac{1}{2} = 6–60$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{\frac{1}{2}} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6$ molecule cm$^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{\frac{1}{2}} \sim 2$ h by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);

hydrolytic $t_{\frac{1}{2}} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

$t_{\frac{1}{2}} = 2$ d for river water, $t_{\frac{1}{2}} < 4$ d for lake water-sediment microcosm, and $t_{\frac{1}{2}} < 100$ d for chemical degradation (hydrolysis) (Gledhill et al. 1980);

biodegradation $t_{\frac{1}{2}} = 19.4$ d in an acclimated shake flask CO$2$ evolution test (Sugatt et al. 1984);
overall $t_{1/2} = 24–168$ h, based on unacclimated river die-away test (Howard et al. 1991)

biodegradation $t_{1/2} = 0.32–3$ d in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48–4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_{1/2} = 9.1$ h in 10% freshwater sediment, and $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Soil: degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

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

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

Biota: depuration $t_{1/2} < 24$ and $> 48$ h (tissues of bluegill sunfish in 21-d exposure, Barrows et al. 1980)

$t_{1/2} < 2$ d from bluegill sunfish (Gledhill et al. 1980; quoted, Versuch 1983).
### 15.1.4 Phosphate Esters

#### 15.1.4.1 Triaryl phosphates

15.1.4.1.1 *t*-Butylphenyl diphenyl phosphate (tBPDP, BPDP)

![Chemical Structure of t-Butylphenyl Diphenyl Phosphate](image)

**Common Name:** *t*-Butylphenyl diphenyl phosphate  
**Synonym:** TBPDP, BPDP

**Chemical Name:**
- **CAS Registry No:** 56803-37-3
  - *o*-tert-butylphenyl diphenyl phosphate (*o*-TBPDP) 83242-23-2  
  - *m*-tert-butylphenyl diphenyl phosphate (*m*-TBPDP) 83242-22-2  
  - *p*-tert-butylphenyl diphenyl phosphate (*p*-TBPDP) 981-40-8

**Molecular Formula:** C_{22}H_{23}O_4P, (CH_3)C_6H_4(C_6H_5)_2O_4P

**Molecular Weight:** 382.389

**Melting Point (°C):**  
- −21 (Muir 1984)

**Boiling Point (°C):**
- 195/0.20 mmHg, 200/0.2 mmHg, 200/0.20 mmHg (*o*-, *m*-, *p*-TBPDP, Wightman & Malaiyanki 1983)  
- 261/6 mmHg (Muir 1984)
- 420 (Boethling & Cooper 1985)

**Density (g/cm³):**
- (Muir 1984)
- 420 (Boethling & Cooper 1985)

**Vapor Pressure (Pa at 25°C):**
- 180 (200°C, Muir 1984)
- 1.87 × 10^{-4} (quoted measured value, Boethling & Cooper 1985)
- 6.13 × 10^{-5} (estimated from boiling point, Boethling & Cooper 1985)

**Henry’s Law Constant (Pa·m³/mol at 25°C):**
- 0.086 (estimated-P/C, Muir 1984, Muir et al. 1985)
- 0.0223, 0.0073 (calculated-P/C, Boethling & Cooper 1985)
- 2.18 (gas stripping, Muir et al. 1985)

**Octanol/Water Partition Coefficient, log K_{ow}:**
- 5.12 (shake flask-conc ratio, Saeger et al. 1979)
- 3.23, 4.76, 6.44; 5.97 (RP-HPLC-k’ correlation; mean value, Renberg et al. 1980)

**Bioconcentration Factor, log BCF:**
- 2.89 (calculated, Saeger et al. 1979)
- 3.36, 3.04, 3.13 (rainbow trout; “initial rate” method, static test, Biofac, Muir et al. 1983b)
- 2.89 (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
- 3.52, 2.89, 2.70 (fathead minnow; “initial rate” method, static test, Biofac, Muir et al. 1983b)
- 2.76 (fathead minnow, calculated with hexane extract, Muir et al. 1983b)
3.94, 2.89  (rainbow trout, fathead minnow, static expt., quoted, Boethling & Cooper 1985)
3.64  (calculated-K_{OC}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
4.16  (calculated-K_{OC}, Muir 1984)
3.36  (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatilization: t_{1/2} = 128 d from 1 m deep water system was estimated to be 128 d (calculated, Muir 1984) moderate rate of volatilization from water, t_{1/2} = 152 d at 0.5-m depth (Muir et al. 1985).

Photolysis:

Oxidation:

Hydrolysis: t_{1/2} = 1.92 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; t_{1/2} < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:
k_{1} = 22.8 h^{-1}, 29.3 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
k_{1} = 17.7 h^{-1}, 18.0 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
k_{2} = 0.0137 h^{-1}, 0.0113 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
k_{2} = 0.0106 h^{-1}, 0.0111 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b)  
k_{2} = 0.0088 h^{-1}, 0.0074 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
k_{2} = 0.0078 h^{-1}, 0.0070 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b)

Half-Lives in the Environment:
Air:
Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; t_{1/2} < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
hydrolysis t_{1/2} = 1.92 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);
t_{1/2} = 128 d, volatilization from 1 m deep water system (Muir 1984);
pseudo-first-order t_{1/2} = 0.44 d in pond water; moderate rate of volatilization from water column with t_{1/2} = 152 d at 0.5-m depth (Muir et al. 1985).

Groundwater:
Sediment: pseudo-first-order t_{1/2} = 39 d in pond bottom sediment during a 49-d period (Muir et al. 1985).
Soil:
Biota: depuration t_{1/2} = 42 h in chironomid larvae (Muir et al. 1985).
15.1.4.1.2  *Cresyl diphenyl phosphate* (CDP)

![Chemical Structure](image)

**Common Name:** Cresyl diphenyl phosphate  
**Synonym:** CDP  
**Chemical Name:**

**CAS Registry No:** 78-31-9  
- *α*-CDP 5254-12-6  
- *m*-CDP 69500-28-3  
- *p*-CDP 78-31-9

**Molecular Formula:** $C_{19}H_{17}O_4P$  
**Molecular Weight:** 340.309  
**Melting Point (°C):**  
- $-40$ (*p*-CDP, Lide 2003)

**Boiling Point (°C):**

- $180/0.60$ mmHg, $190/0.60$ mmHg, $200/0.70$ mmHg (*α*-*, m-*-, *p*-CDP, Wightman & Malaiyandi 1983)  
- $368, 390$ (at 1 atm, Boethling & Cooper 1985)  
- $235–255/4$ mmHg, $255/5$ mmHg (Boethling & Cooper 1985)

**Density (g/cm³ at 20°C):**

**Molar Volume (cm³/mol):**

**Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):**

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

**Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:**

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

- 2.60 (shake flask-GC, Saeger et al. 1979)

**Vapor Pressure (Pa at 25°C):**

- $5.47 \times 10^{-3}$, $1.21 \times 10^{-3}$, $3.87 \times 10^{-4}$, $2.80 \times 10^{-4}$ (estimated from reported boiling points, Boethling & Cooper 1985)  
- $6.27 \times 10^{-4}$ (quoted measured value, Boethling & Cooper 1985)

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

- 0.470 (calculated-P/C, Muir 1984)  
- 0.798, 0.162, 0.0820, 0.0507, 0.0355 (calculated-P/C, Boethling & Cooper 1985)

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

- 4.505 (shake flask-concn ratio, Saeger et al. 1979)  
- 3.23, 3.63, 4.06; 3.77 (RP-HPLC-k’ correlation; mean value, Renberg 1980)  
- 4.40 (Bengtsson et al. 1986)

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

**Bioconcentration Factor, log $BCF$:**

- 2.56 (calculated, Saeger et al. 1979)  
- 2.99 (calculated-$K_{OW}$, Boethling & Cooper 1985)  
- 2.002.34 (bleak, 280-d exposure, Bengtsson et al. 1986)
Sorption Partition Coefficient, log $K_{OC}$:

- 3.83 (calculated-$K_{OW}$, Muir 1984)
- 3.41 (soil, estimated from solubility, Boethling & Cooper 1985)

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

- Volatilization: $t_{1/2} \approx 22$ d for 1 m deep water system (estimated, Muir 1984).
- Photolysis:
- Oxidation:
- Hydrolysis:
- Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air:
  - Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
  - volatilization $t_{1/2} = 22$ d for 1 m deep water system (estimated, Muir 1984).
- Groundwater:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 4$ d or less (beak, 28-d exposure, Bengtsson 1986).
15.1.4.1.3 Isopropylphenyl diphenyl phosphate (IPPDP)

Common Name: Isopropylphenyl diphenyl phosphate
Synonym: IPPDP, IPDP
Chemical Name:
CAS Registry No: 28108-99-8
\(\alpha\)-IPPDP 64532-94-1
\(m\)-IPPDP 69515-46-4
\(p\)-IPPDP 55864-04-5
Molecular Formula: \(C_{21}H_{21}O_4P, (CH_3)\_2CHC_6H_4O_4P\)
Molecular Weight: 368.362
Melting Point (°C): 
\(-26\) (Muir 1984)
Boiling Point (°C):
175/0.05 mmHg, 180/0.02 mmHg, 185/0.05 mmHg (Wightman & Malaiyandi 1983)
220–230/1 mmHg (Muir 1984, Boethling & Cooper 1985)
Density (g/cm\(^3\) at 20°C):
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 (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
\(2.20\) (room temp, shake flask-GC, Saeger et al. 1979)
Vapor Pressure (Pa at 25°C):
\(1.47 \times 10^{-4}\) (estimated from boiling point, Boethling & Cooper 1985)
\(3.73 \times 10^{-5}\) (quoted measured value, Boethling & Cooper 1985)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
\(0.243, 0.0628\) (calculated-P/C, Boethling & Cooper 1985)
Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
\(5.305\) (shake flask-concn ratio, Saeger et al. 1979; quoted, Muir 1984)
\(3.23, 4.30, 5.40, 6.57; 5.99\) (RP-HPLC-\(k’\) correlation; mean, Renberg et al. 1980)
\(5.70\) (quoted measured value, Boethling & Cooper 1985)
Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):
Bioconcentration Factor, log BCF:
\(2.99\) (calculated, Saeger et al. 1979)
\(3.88\) (estimated from solubility, Boethling & Cooper 1985)
Sorption Partition Coefficient, log \(K_{\text{oc}}\):
\(4.26\) (calculated-\(K_{\text{ow}}\), Muir 1984)
\(3.45\) (soil, estimated from solubility, Boethling & Cooper 1985)
Environmental Fate Rate Constants, \(k\), or Half-Lives, \(t_{1/2}\):
Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of water; \( t_{1/2} = 28–48 \) d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

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

Half-Lives in the Environment:
Air:
Surface water: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of the water; \( t_{1/2} = 28–48 \) d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Groundwater:
Sediment:
Soil:
Biota:
**15.1.4.1.4 4-Cumylphenyl diphenyl phosphate (CPDPP)**

![Chemical Structure](image)

Common Name: 4-Cumylphenyl diphenyl phosphate  
Synonym: CPDPP  
Chemical Name:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>CAS Registry No:</td>
<td>84602-56-2</td>
</tr>
<tr>
<td>Molecular Formula:</td>
<td>$C_{27}H_{25}O_4P, C_6H_5C(CH_3)_2(C_6H_5)_2O_4P$</td>
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<td>Molecular Weight:</td>
<td>444.458</td>
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<td>Melting Point (°C):</td>
<td>230–235/0.15 mmHg (Wightman &amp; Malaiyandi 1983)</td>
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<td>Boiling Point (°C):</td>
<td>494 (Boethling &amp; Cooper 1985)</td>
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<tr>
<td>Density (g/cm³ at 20°C):</td>
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<tr>
<td>Molar Volume (cm³/mol):</td>
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<tr>
<td>Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):</td>
<td></td>
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<tr>
<td>Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):</td>
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</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:</td>
<td></td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C):</td>
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<td></td>
<td>0.063 ± 0.025 (Mayer et al. 1981)</td>
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<td></td>
<td>0.060 (Boethling &amp; Cooper 1985)</td>
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<tr>
<td>Vapor Pressure (Pa at 25°C):</td>
<td>$1.726 \times 10^{-9}$ (estimated from boiling point, Boethling &amp; Cooper 1985)</td>
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<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C):</td>
<td>$8.62 \times 10^{-4}$ (calculated-P/C, Boethling &amp; Cooper 1985)</td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:</td>
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<tr>
<td></td>
<td>6.08 (Mayer et al. 1981)</td>
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<td>6.10 (quoted, Boethling &amp; Cooper 1985)</td>
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<tr>
<td>Octanol/Air Partition Coefficient, log $K_{\text{OA}}$:</td>
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<td>Bioconcentration Factor, log BCF:</td>
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<td>3.40 (calculated-$K_{\text{OW}}$, Mayer et al. 1981)</td>
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<td></td>
<td>4.40 (calculated-$K_{\text{OW}}$, Boethling &amp; Cooper 1985)</td>
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<tr>
<td>Sorption Partition Coefficient, log $K_{\text{OC}}$:</td>
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<td></td>
<td>4.53 (soil, calculated-$S$ and $K_{\text{OW}}$, Mayer et al. 1981)</td>
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<tr>
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<td>4.30 (soil, estimated from solubility, Boethling &amp; Cooper 1985)</td>
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**Environmental Fate Rate Constants, k, or Half-Lives, $t_{\frac{1}{2}}$:**

<table>
<thead>
<tr>
<th>Process</th>
<th>Value</th>
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<tbody>
<tr>
<td>Volatilization:</td>
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<td>Photolysis:</td>
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<td>Oxidation:</td>
<td></td>
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</tbody>
</table>
Hydrolysis: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: $t_{1/2} > 21$ d in river die-away procedure; the half-lives of the disappearance by sediment adsorption and degradation of CPDF for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d, sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Biotransformation:

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

Half-Lives in the Environment:

Air:
Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7; biodegradation $t_{1/2} > 21$ d in river die-away procedure (Mayer et al. 1981).

Groundwater:
Sediment: rapidly disappeared from the active core-water columns, 90% in < 3 d in the microcosm-lake simulation study, the half-lives of the disappearance of CPDF by sediment adsorption and degradation are, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:

Biota:
15.1.4.1.5  *Nonylphenyl diphenyl phosphate (NPDPP)*

![Chemical structure of NPDPP](image)

Common Name: Nonylphenyl diphenyl phosphate  
Synonym: NPDPP, Pydral 50E  
Chemical Name:  
CAS Registry No: 38638-05-0  
   - *m*-NPDPP  84602-55-1  
   - *p*-NPDPP  64532-97-4  
Molecular Formula: C_{27}H_{33}O_{4}P, C_{9}H_{19}(C_{6}H_{5})_{3}O_{4}P
Molecular Weight: 452.522  
Melting Point (°C):  
Boiling Point (°C):  
   - 220–225/0.07 mmHg (*m*-NPDPP, Wightman & Malaiyandi 1983)  
   - 215–220/0.07 mmHg (*p*-NPDPP, Wightman & Malaiyandi 1983)  
   - 471  (Boethling & Cooper 1985)  
Density (g/cm³ at 20°C):  
Molar Volume (cm³/mol):  
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):  
Entropy of Fusion, ΔS_{fus} (J/mol K):  
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:  
Water Solubility (g/m³ or mg/L at 25°C):  
   - 0.77 ± 0.25  (Mayer et al. 1981)  
   - 0.80  (Boethling & Cooper 1985)  
Vapor Pressure (Pa at 25°C):  
   - 6.13 × 10⁻⁵ (estimated from boiling point, Boethling & Cooper 1985)  
Henry’s Law Constant (Pa·m³/mol at 25°C):  
   - 0.00142  (calculated-P/C, Boethling & Cooper 1985)  
Octanol/Water Partition Coefficient, log K_{ow}:  
   - 5.93  (Mayer et al. 1981; quoted, Muir 1984)  
   - 5.90  (quoted, Boethling & Cooper 1985)  
Octanol/Air Partition Coefficient, log K_{oa}:  
Bioconcentration Factor, log BCF:  
   - 3.32  (estimated, Mayer et al. 1981)  
   - 2.84, 2.49–2.96  (mean value and range, rainbow trout 90-d exposure, Mayer et al. 1981)  
   - 4.26  (calculated-K_{ow}, Boethling & Cooper 1985)  
Sorption Partition Coefficient, log K_{oc}:  
   - 4.36  (soil, calculated-solubility and K_{ow}, Mayer et al. 1981)  
   - 4.61  (calculated-K_{ow}, Muir 1984)  
   - 3.69  (soil, estimated from solubility, Boethling & Cooper 1985)  
Environmental Fate Rate Constants, k, Half-Lives, t\(_{1/2}\):  
Volatilization:  
Photolysis:
Oxidation:
Hydrolysis: $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).
Biodegradation: primary biodegradation $t_{1/2} > 21$ d in river die-away procedure; half-life for disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

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

Half-Lives in the Environment:
Air:
Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Groundwater:
Sediment: rapidly disappeared from the active core-water column, 90% in < 3 d. Time to 50% disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark – $t_{1/2} < 3$ d; sterile, aerated, light – $t_{1/2} = 7$ d and sterile, nitrogen-purge, light – $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:
Biota:
15.1.4.1.6 **Triphenyl phosphate (TPP)**

![Triphenyl phosphate structure]

**Common Name:** Triphenyl phosphate  
**Synonym:** TPP  
**Chemical Name:** triphenyl phosphate  
**CAS Registry No:** 115-86-6  
**Molecular Formula:** C\textsubscript{18}H\textsubscript{15}O\textsubscript{4}P  
**Molecular Weight:** 326.283  
**Melting Point (°C):**  
\[50.5\] (Lide 2003)  
**Boiling Point (°C):**  
\[245/11 \text{ mmHg}\] (Verschueren 1983; Budavari 1989; Lide 2003)  
\[377\] (Stephenson & Malanowski 1987)  
**Density (g/cm\textsuperscript{3}):**  
270.7  
50°C, Stephenson & Malanowski 1987)  
**Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):**  
**Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):**  
**Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F: 0.27, 0.292  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):**  
\[1.90\] (shake flask-GC, Saeger et al. 1979)  
\[1.9 \pm 0.2\] (Mayer et al. 1981)  
\[0.73\] (shale flask-nephelometry, Hollifield 1979)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
\[< 13.3\] (30°C, Verschueren 1983)  
\[2.0 \times 10^{-4}, 1.6 \times 10^{-4}, 1.07 \times 10^{-4}\] (estimated from reported boiling points, Boethling & Cooper 1985)  
\[\log (P/\text{Pa}) = 8.195 – 4253/(T/K);\] temp range 275–410°C (Antoine eq., Stephenson & Malanowski 1987)  
\[\log (P/\text{mmHg}) = 28.0972 – 5.6684 \times 10^{-3}/(T/K) – 5.9768 \log (T/K) – 3.1567 \times 10^{-6}/(T/K)^2;\] temp range 323–687 K (vapor pressure eq., Yaws et al. 1994)  
**Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):**  
0.168  
0.0265, 0.0284, 0.018  
(calculated-P/C, Muir 1984)  
(calculated-P/C, Boethling & Cooper 1985)  
**Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):**  
4.63  
4.62  
4.78  
3.15  
3.63–3.61  
4.60, 4.70  
3.90  
(shake flask-conc ratio, Saeger et al. 1979)  
(Mayer et al. 1981)  
(shake flask-conc ratio, Sasaki et al. 1981)  
(RP-HPTLC-\(k'\) correlation, Renberg et al. 1980)  
(literature average, Muir 1984)  
(Boethling & Cooper 1985)  
(Bengtsson et al. 1986)  
**Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):**  
**Bioconcentration Factor, log BCF or log \(K_{\text{b}}\):**  
2.45, 2.62  
2.22  
(quoted-rainbow trout data, calculated-\(K_{\text{ow}}\), Saeger et al. 1979)  
(fathead minnow, mixed isomers, Veith et al. 1979)
3.41 (rainbow trout, rate constant ratio $k_1/k_2$, Muir et al. 1980)
3.29, 2.63, 2.58 (rainbow trout, calculated-$K_{OW}$, Muir et al. 1980)
3.02, 2.92, 2.00 (rainbow trout, calculated-$S$, Muir et al. 1980)
2.62 (rainbow trout, estimated from $K_{OW}$, Mayer et al. 1981)
2.43, 2.12–2.56 (mean value, range, rainbow trout in 90-d exposure, Mayer et al. 1981)
2.40–2.79 (killifish, whole fish basis, 72-h exposure, static system, Sasaki et al. 1981)
2.04–2.18 (goldfish, static system, Sasaki et al. 1981; quoted, Boethling & Cooper 1985)
2.20–2.79 (killifish, flow through system, Sasaki et al. 1982; quoted, Boethling & Cooper 1985)
2.28–2.29 (killifish, 32–35 d exposure, flow through system, Sasaki et al. 1983)
3.14, 2.76, 2.96 (rainbow trout: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.51 (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.24, 2.75, 2.34 (fathead minnow: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.62 (fathead minnow, calculated with hexane extract, Muir et al. 1983b)
2.76, 2.51 (rainbow trout in static test exppt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
2.75, 2.62 (fathead minnow in static test exppt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
3.26 (estimated-$K_{OW}$, Boethling & Cooper 1985)
2.60 (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log $K_{OC}$:
3.74 (soil, calculated-$S$, $K_{OW}$, Mayer et al. 1981)
3.89 (calculated-$K_{OW}$, Muir 1984)
3.49 (calculated-solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constant, $k$, and Half-Lives, $t_1/2$:
Volatilization: $t_1/2 = 60$ d (Muir 1984).
Photolysis:
Oxidation:
Hydrolysis:

$k = 0.0253$ and $0.0227$ L mol$^{-1}$ s$^{-1}$ for the colorimetric and acid-base method, respectively, in dioxan-water
(3:1 v/v) at 35°C; the mean second order rate constants: $10^3 k_2$ at 0°C, 10.1°C, 24.7°C, and 35°C were
0.235, 0.477, 1.06, and 2.32 L mol$^{-1}$ s$^{-1}$, respectively, in 60% dioxan-water (Barnard et al. 1961);
$t_1/2 = 1.3$ yr under neutral conditions from kinetic data in the environment (estimated, Saeger et al. 1979)
$k = 6.0 \times 10^{-8}$ s$^{-1}$, with $t_1/2 = 130$ d, the pseudo-first-order rate constant in dioxan-water (3:1 v/v) at 100°C;
while the second-order rate constant $k = 0.0106$ L mol$^{-1}$ s$^{-1}$ with $t_1/2 = 23$ d at pH 9.5 and $t_1/2 = 474$ d at
pH 8.2 under alkaline conditions at 24.7°C (estimated, Howard & Deo 1979);
$k$(second order alkaline) = 0.027 M$^{-1}$ s$^{-1}$, with an estimated $t_1/2 \sim$ 1000 yr (Wolfe 1980)
$t_1/2 = 19$ d at pH 7 but $t_1/2 = 3$ d at pH 9 at 25°C, the most important process for abiotic transformation of
aryl phosphates in the environment, much more rapid at alkaline than at neutral pH (Mayer et al. 1981, quoted,
Boethling & Cooper 1985)
$t_1/2 = 7.5$ d at pH 8.2, $t_1/2 = 1.3$ d at pH 9.5, $t_1/2 = 20–25$ d at pH 7 and 21°C (Howard & Deo 1979; quoted,
Boethling & Cooper 1985)
$t_1/2 = 0.49$ h at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b)

Biodegradation: complete primary degradation in less than 7 d in the river die-away studies exposed to the
natural microbial population of the river water; $t_1/2 < 7$ d for primary biodegradation rate for from semicon-
tinuous activated sludge studies (Saeger et al. 1979);
readily biodegraded, in the semicontinuous activated sludge test, degradation of TPP exceeding 95% was
observed over a 24-h cycle, and river die-away tests showed $t_1/2 = 2–4$ d; time to 50% from the active
core water-column disappearance for TPP in microcosms simulating lake conditions was 3–10 d (Mayer

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

$k_1 = 46.36$ h$^{-1}$ (rainbow trout, Muir et al. 1980).
$k_2 = 0.0197$ h$^{-1}$ (rainbow trout, 0–9 d, fast clearance, Muir et al. 1980).
$k_3 = 0.00245$ h$^{-1}$ (rainbow trout, 9–31 d, slow clearance, Muir et al. 1980).
k₁ = 0.4–0.6 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)
k₁ = 2.1–4.2 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)
k₁ = 3.3–10.4 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)
k₁ = 3.3–16.9 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)
k₂ = 0.023 h⁻¹ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concn decay curve, Muir et al. 1983)
k₂ = 0.039 h⁻¹ (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)
k₂ = 0.011 h⁻¹ (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)
k₂ = 0.016 h⁻¹ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983).
k₁ = 22.7 h⁻¹, 20.7 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
k₁ = 16.5 h⁻¹, 14.5 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
k₂ = 0.0116 h⁻¹, 0.0144 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b)
k₂ = 0.0121 h⁻¹, 0.0140 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
k₂ = 0.0076 h⁻¹, 0.0107 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b)

**Half-Lives in the Environment:**

**Air:**
Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; t₁/₂ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
t₈ = 5 h in the water containing killifish and over 100 h for goldfish (Sasaki et al. 1981);
hydrolysis t₈₁ = 19 d at pH 7 but t₈₂ = 3 d at pH 9; t₈₃ = 2–4 d in river die-away test at 25°C, (Mayer et al. 1981, quoted, Boethling & Cooper 1985);
t₈₄ = 7.5 d at pH 8.2 and t₈₅ = 1.3 d at pH 9.5, t₈₆ = 20–25 d at pH 7 at 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985);
estimated hydrolysis t₈₇ ~ 10³ yr (Wolfe 1980);
volutilization t₈₈(calc) = 60 d for 1 m deep water(Muir 1984).

**Ground water:**
Sediment: water-column disappearance t₈₉ ~ 3 d of TPP by both adsorption and degradation from microcosms-lake simulation study, for the microcosm core conditions: active, aerated, light or dark – t₈₉ = 3 d; active, nitrogen-purge, light – t₈₉ = 3 d; sterile, aerated, light – t₈₉ = 7 d and sterile, nitrogen-purge, light – t₈₉ = 10 d (Mayer et al. 1981).

**Soil:**
Biota: elimination t₈₉ = 30.4 h in pond sediment-water, t₈₉ = 17.6 h in river water, t₈₉ = 62.7 h in river sediment-water, t₈₉ = 44.4 in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983a); elimination t₈₉ = 4 d or less (bleak, 28-d exposure, Bengtsson et al. 1986).
15.1.4.1.7 Tricresyl phosphate (TCP)

Common Name: Tricresyl phosphate
Synonym: TCP, tritolyl phosphate, tris(methylphenyl) phosphate
Chemical Name: phosphoric acid tris(methylphenyl) ester

- o-TCP: tris(2-methylphenyl) phosphate; phosphoric acid tri(2-tolyl) ester
- m-TCP: tris(3-methylphenyl) phosphate; phosphoric acid tri(3-tolyl) ester
- p-TCP: tris(4-methylphenyl) phosphate; phosphoric acid tri(4-tolyl) ester

CAS Registry No:
- o-TCP [78-30-8]; m-TCP [563-04-2]; p-TCP [78-32-0]
- mixed isomers - tris(methylphenyl) phosphate [1330-78-5]

Molecular Formula: C_{21}H_{21}O_4P, (CH_3C_6H_4)_3O_4P
Molecular Weight: 368.362

Melting Point (°C):
- –25/–30 (o-TCP, Verschueren 1983)
- –33 (mixed isomers, Riddick et al. 1986)
- 11, 25–26, 77–8 (o-TCP, m-TCP, p-TCP, Muir 1984)
- 11, 25, 77.5 (o-TCP, m-TCP, p-TCP, Stephenson & Malanowski 1987)
- 11, 25.5, 77.5 (o-TCP, m-TCP, p-TCP, Lide 2003)

Boiling Point (°C):
- 201/1 mmHg (commercial quality, Burrow 1946)
- 420 (o-TCP, Verschueren 1983)
- 410 (o-TCP, Muir 1984; Lide 2003)
- 313, 216–216/0.5 mmHg (mixed isomers, o-, m-TCP, Riddick et al. 1986)
- 241–255/4 mmHg, 265/5 mmHg (Boethling & Cooper 1985)

Density (g/cm³ at 20°C):
- 1.159, 1.1718 (25°C, mixture of isomers, o-TCP, Riddick et al. 1986)
- 1.16 (o-TCP, Verschueren 1983; Riddick et al. 1987; Budavari 1989)

Molar Volume (cm³/mol):
- 308.1 (20°C, calculated-density, Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ∆H_v (kJ/mol):
- 116.3, 102.9, 113 (m-TCP, Small et al. 1948)
- 113.4 (p-TCP, Small et al. 1948)

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: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 0.40 (shake flask-GC, Saeger et al. 1979)
- 0.074 (p-TCP practical grade, shake flask-nephelometry; Hollifield 1979)
- 0.36 (mixed isomers, Muir 1984)
- < 0.10 (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):
- 0.00516–0.00612* (m-TCP, Celluloid Corporation samples at 80°C, static and dynamic methods, measured range 80–136°C, Verhoek & Marshall 1939)
- log (P/µmHg) = 15.886 – 6088/(T/K); temp range 80–136°C (m-TCP, Celluloid Corporation samples, static and dynamic methods, Verhoek & Marshall 1939)
0.0132* \((m\text{-TCP, Eastman Kodak Co. samples at 85.2}^\circ\text{C, static and dynamic methods, measured range 85.2–126}^\circ\text{C, Verhoe & Marshall 1939})\)

\[ \log (P/\mu\text{mHg}) = 13.982 - \frac{5373}{(T/K)}; \text{ temp range 85.2–126}^\circ\text{C} \]

\((m\text{-TCP, Eastman Kodak Co. samples at 85.2}^\circ\text{C, static and dynamic methods, measured range 85.2–126}^\circ\text{C, Verhoe & Marshall 1939})\)

\[ \log (P/\mu\text{mHg}) = 15.223 - \frac{5926}{(T/K)}; \text{ temp range 92–145}^\circ\text{C} \]

\((p\text{-TCP, static and dynamic methods, Verhoe & Marshall 1939})\)

\[ 4.13 \times 10^{-4} \text{ (extrapolated from extpl. data, measured range 140–156}^\circ\text{C, commercial quality, ebulliometry, Burrows 1946}) \]

\[ \log (P/\mu\text{mHg}) = 12.69 - \frac{5925}{(T/K)}; \text{ temp range: } -100–150^\circ\text{C (Antoine eq. from extpl., effusion, technical grade, Small et al. 1948)} \]

\[ \log (P/\mu\text{mHg}) = 10.98 - \frac{5373}{(T/K)}; \text{ Antoine eq. from literature, Small et al. 1948) } \]

\[ \log (P/\mu\text{mHg}) = 12.22 - \frac{5895}{(T/K)}; \text{ temp range: 100–150}^\circ\text{C (m-TCP, Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948) } \]

\[ \log (P/\mu\text{mHg}) = 12.22 - \frac{5926}{(T/K)}; \text{ Antoine eq., Small et al. 1948) } \]

\[ \log (P/mmHg) = 15.223 - \frac{5926}{(T/K)}; \text{ temp range 85.2–126}^\circ\text{C} \]

\((m\text{-TCP, Eastman Kodak Co. samples, static and dynamic methods, Verhoek & Marshall 1939})\)

\[ \log (P/mmHg) = 13.982 - \frac{5373}{(T/K)}; \text{ temp range 85.2–126}^\circ\text{C} \]

\[ \log (P/mmHg) = 14.12 - \frac{5480}{(T/K)}; \text{ temp range 115–168}^\circ\text{C} \]

\((p\text{-TCP, pendulum-tensimeter method, Perry & Weber 1949})\)

\[ \log (P/mmHg) = -0.2185 \times 20835.9/(T/K) + 10.654252; \text{ temp range 154.6–313}^\circ\text{C (tritolyl phosphate, Antoine eq., Weast 1972–73)} \]

\[ \log (P/kPa) = 11.81 - \frac{5925}{(T/K)}; \text{ temp range 293–700 K (o-TCP, Antoine eq., Riddick et al. 1986)} \]

\[ \log (P/kPa) = 10.67 - \frac{5787}{(T/K)}; \text{ temp range 293–700 K (m-TCP, Antoine eq., Riddick et al. 1986)} \]

\[ \log (P/kPa) = 13.24 - \frac{5480}{(T/K)}; \text{ temp range 293–700 K (p-TCP, Antoine eq., Riddick et al. 1986)} \]

\[ \log (P/kPa) = 8.56 - \frac{4535}{(T/K)}; \text{ temp range 293–700 K (o-TCP, Antoine eq., Stephenson & Malanowski 1987)} \]

\[ \log (P/kPa) = 11.8856 - \frac{6104.5}{[(T/K) - 10.81]}; \text{ temp range 398–530 K (m-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)} \]

\[ \log (P/kPa) = 10.245 - \frac{5480}{(T/K)}; \text{ temp range 388–530 K (p-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)} \]

\[ 3.07 \times 10^{-4}, 1.25 \times 10^{-4} \text{ (estimated from reported boiling points, Boething & Cooper 1985)} \]

\[ 1.87 \times 10^{-4} \text{ (quoted measured value, Boethling & Cooper 1985)} \]

\[ 6.10 \times 10^{-6} \text{ (liquid P, GC-RT correlation, Hinckley et al. 1990)} \]

\[ \log (P/mmHg) = 21.1624 - \frac{5.2756 \times 10^3}{(T/K)} - 3.3565 \cdot \log(T/K) + 8.666 \times 10^{-6} \cdot (T/K) - 2.9202 \times 10^{-9} \cdot (T/K)^2; \text{ temp range 428–566 K (o-TCP, vapor pressure eq., Yaws et al. 1994)} \]

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

0.0218 \(\text{ (calculated-P/C, Muir 1984, Muir et al. 1985)}\)

0.283, 0.172, 0.111 \(\text{ (calculated-P/C, Boethling & Cooper 1985)}\)

8.38 \(\text{ (m-TCP, gas stripping, Muir et al. 1985)}\)

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

3.42 \(\text{ (HPLC-RT correlation, Veith 1979)}\)

5.11 \(\text{ (shake flask-concn ratio, Saeger et al. 1979)}\)

4.30, 4.65; 4.50 \(\text{ (RP-HPTLC-k’ correlation, Renberg et al. 1980)}\)

5.10–5.12 \(\text{ (Muir 1984)}\)

5.10–5.30 \(\text{ (Bengtsson et al. 1986)}\)

Bioconcentration Factor, log \(BCF\):

5.505, 4.45, 3.57, 3.57, 3.46 \(\text{ (p-TCP, ecological magnification factors for alga, snail, mosquito, fish and } Daphnia, \text{ Metcalf 1976)}\)

2.88 \(\text{ (calculated for rainbow trout, Saeger et al. 1979)}\)

2.22 \(\text{ (fathead minnow, 32-d exposure, Veith et al. 1979)}\)

3.44, 3.15, 3.17 \(\text{ (p-TCP for rainbow trout: “initial rate” method, static test, Biofac, Muir et al. 1983b)}\)
2.89 \( (p\text{-TCP for rainbow trout, calculated with hexane extract, Muir et al. 1983b})
\)

3.34, 2.97, 2.77 \( (p\text{-TCP for fathead minnow: “initial rate” method, static test, Biofac, Muir et al. 1983b})
\)

2.85 \( (p\text{-TCP, fathead minnow, calculated with hexane extractable radioactivity, Muir et al. 1983b})
\)

3.07, 2.89, 3.04 \( (m\text{-TCP for rainbow trout: “initial rate” method, static test, Biofac, Muir et al. 1983b})
\)

2.49 \( (m\text{-TCP for rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b})
\)

3.22, 2.77, 2.59 \( (m\text{-TCP for fathead minnow: “initial rate” method, static test, Biofac, Muir et al. 1983b})
\)

2.66 \( (m\text{-TCP, fathead minnow, calculated with hexane extract, Muir et al. 1983b})
\)

3.15, 2.89; 3.64 \( (rainbow trout: p\text{-, m-TCP, static expt.; estimated-K\textsubscript{OW}, Boethling & Cooper 1985})
\)

2.60 \( (bleak, 28-d exposure, Bengtsson et al. 1986)
\)

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

4.44 \( (\text{calculated-K\textsubscript{OW}, Muir 1984})
\)

3.86 \( (\text{estimated from solubility, Boethling & Cooper 1985})
\)

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

Volatilization: \( t_{\frac{1}{2}} = 496 \text{ d} \) (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis: \( t_{\frac{1}{2}} = 73 \text{ d and 52 d at } 22^\circ\text{C for aryl phosphates (75% TCP and 18% TXP) in demineralized and}
\)

river water (Wagemann et al. 1974; quoted, Boethling & Cooper 1985);

degradation \( t_{\frac{1}{2}} = 3-4 \text{ d for } o\text{-, m-TCP and 5 d for } p\text{-TCP in Lake Ontario water (Howard & Dao 1979})
\)

second order alkaline hydrolysis rate constant \( k = 0.025 \text{ M}^{-1} \text{s}^{-1} \) (estimated, \( p\text{-TCP, Wolfe 1980})
\)

\( t_{\frac{1}{2}} = 1.31 \text{ h, 1.66 h for } m\text{-TCP and } p\text{-TCP, respectively, at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b})
\)

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the

natural microbial population of the water; \( t_{\frac{1}{2}} < 7 \text{ d for primary biodegradation rate from semicontinuous}
\)

activated sludge studies (Saeger et al. 1979);

Biotransformation:

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

For \( p\text{-TCP} \):

\( k_1 = 25.8 \text{ h}^{-1}, 21.8 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L, Muir et al. 1983b})
\)

\( k_1 = 15.9 \text{ h}^{-1}, 7.80 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L, Muir et al. 1983b})
\)

\( k_2 = 0.0104 \text{ h}^{-1}, 0.00963 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L for 0–144 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0106 \text{ h}^{-1}, 0.0133 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L for 0–432 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0096 \text{ h}^{-1}, 0.0077 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L for 0–144 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0070 \text{ h}^{-1}, 0.0095 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L for 0–432 h interval, Muir et al. 1983b})
\)

For \( m\text{-TCP} \):

\( k_1 = 28.8 \text{ h}^{-1}, 24.0 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L, Muir et al. 1983b})
\)

\( k_1 = 18.2 \text{ h}^{-1}, 12.2 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L, Muir et al. 1983b})
\)

\( k_2 = 0.0242 \text{ h}^{-1}, 0.0229 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L for 0–144 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0115 \text{ h}^{-1}, 0.0149 \text{ h}^{-1} \) (rainbow trout, exposure concn 5, 50 \( \mu \text{g/L for 0–432 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0147 \text{ h}^{-1}, 0.0117 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L for 0–144 h interval, Muir et al. 1983b})
\)

\( k_2 = 0.0085 \text{ h}^{-1}, 0.0101 \text{ h}^{-1} \) (fathead minnow, exposure concn 5, 50 \( \mu \text{g/L for 0–432 h interval, Muir et al. 1983b})
\)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the

natural microbial population of the water; \( t_{\frac{1}{2}} < 7 \text{ d for primary biodegradation rate from semicontinuous}

activated sludge studies (Saeger et al. 1979);

degradation \( t_{\frac{1}{2}} = 3-4 \text{ d for } o\text{-, m-TCP and } t_{\frac{1}{2}} = 5 \text{ d for } p\text{-TCP in Lake Ontario water (Howard & Dao 1979}}
\)

\( t_{\frac{1}{2}} = 1.66 \text{ h and 1.31 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b})
\)

volatilization \( t_{\frac{1}{2}}\text{(calc)} = 296 \text{ d in 1 m deep water system (Muir 1984})
\)

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pseudo-first-order $t_{1/2} = 0.57$ d in pond water; moderate volatilization from water column with $t_{1/2} = 84$ d at 0.5-m depth (Muir et al. 1985).

Groundwater:
Sediment: $t_{1/2} = 39$ d in bottom sediment of a small pond (Muir et al. 1985).

Soil:
Biota: depuration $t_{1/2} = 135$ h in chironomid larvae (Muir et al. 1985);
elimination $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

**TABLE 15.1.4.1.7.1**
Reported vapor pressures of tricresyl phosphate at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>tri-\textit{m}-cresyl phosphate</th>
<th>Verhoek &amp; Marshall 1939</th>
</tr>
</thead>
<tbody>
<tr>
<td>static and dynamic methods</td>
<td></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>P/Pa</td>
</tr>
<tr>
<td>80</td>
<td>0.00612</td>
</tr>
<tr>
<td>80</td>
<td>0.00604</td>
</tr>
<tr>
<td>80</td>
<td>0.00516</td>
</tr>
<tr>
<td>90</td>
<td>0.0177</td>
</tr>
<tr>
<td>100.2</td>
<td>0.0461</td>
</tr>
<tr>
<td>109.9</td>
<td>0.1233</td>
</tr>
<tr>
<td>110.5</td>
<td>0.1276</td>
</tr>
<tr>
<td>114.0</td>
<td>0.212</td>
</tr>
<tr>
<td>114.0</td>
<td>0.208</td>
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<tr>
<td>114.0</td>
<td>0.213</td>
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<tr>
<td>119.0</td>
<td>0.323</td>
</tr>
<tr>
<td>120.0</td>
<td>0.315</td>
</tr>
<tr>
<td>120.7</td>
<td>0.316</td>
</tr>
<tr>
<td>124.0</td>
<td>0.492</td>
</tr>
<tr>
<td>124.0</td>
<td>0.504</td>
</tr>
<tr>
<td>125.9</td>
<td>0.509</td>
</tr>
<tr>
<td>128.8</td>
<td>0.739</td>
</tr>
<tr>
<td>129.0</td>
<td>0.785</td>
</tr>
<tr>
<td>130.0</td>
<td>0.777</td>
</tr>
<tr>
<td>131.0</td>
<td>0.809</td>
</tr>
<tr>
<td>136.2</td>
<td>1.352</td>
</tr>
<tr>
<td>eq. 1</td>
<td>P/μmHg</td>
</tr>
<tr>
<td>A</td>
<td>15.886</td>
</tr>
<tr>
<td>B</td>
<td>6088</td>
</tr>
<tr>
<td>(\Delta H_v = 116.54 \text{ kJ/mol})</td>
<td></td>
</tr>
</tbody>
</table>

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<tr>
<th>tri-\textit{p}-cresyl phosphate</th>
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<td>114.0</td>
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</tr>
<tr>
<td>(\Delta H_v = 116.54 \text{ kJ/mol})</td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 15.1.4.1.7.1a Logarithm of vapor pressure versus reciprocal temperature for tris(m-cresyl) phosphate.

FIGURE 15.1.4.1.7.1b Logarithm of vapor pressure versus reciprocal temperature for tris(p-cresyl) phosphate.
15.1.4.1.8  *Trixylenyl phosphate (TXP)*

![Chemical Structure](image)

Common Name: Trixylenyl phosphate  
Synonym: TXP  
Chemical Name:  
CAS Registry No: 25155-23-1  
Molecular Formula: C\textsubscript{24}H\textsubscript{27}O\textsubscript{4}P, [(CH\textsubscript{3})\textsubscript{2}C\textsubscript{6}H\textsubscript{3}]\textsubscript{3}O\textsubscript{4}P  
Molecular Weight: 410.442  
Melting Point (°C):  
−20  (mixed isomers, Muir 1984)  
Boiling Point (°C):  
261  (at 6 mmHg, Muir 1984)  
225–295/6 mmHg, 248–265/4 mmHg, 270/3 mmHg (Boethling & Cooper 1985)  
Density (g/cm\textsuperscript{3} at 20°C):  
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):  
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:  
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):  
0.89  (shake flask-GC, Saeger et al. 1979)  
0.89  (mixed isomers, Muir 1984)  
Vapor Pressure (Pa at 25°C):  
$7.20 \times 10^{-4}$, $1.47 \times 10^{-4}$, $3.067 \times 10^{-5}$  (estimated from reported boiling points, Boethling & Cooper 1985)  
$6.93 \times 10^{-6}$  (30°C, Boethling & Cooper 1985)  
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):  
0.334, 0.0689, 0.0142, 0.00314  (calculated-P/C, Boethling & Cooper 1985)  
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:  
5.63  (shake flask-concn ratio, Saeger et al. 1979)  
5.26  (RP-HPTLC-$k'$ correlation, Renberg et al. 1980)  
5.63  (Muir 1984)  
5.70  (Boethling & Cooper 1985)  
6.40–6.60  (Bengtsson et al. 1986)  
Bioconcentration Factor, log $BCF$:  
3.15  (calculated for rainbow trout, Saeger et al. 1979)  
4.04  (estimated from $K_{\text{ow}}$, Boethling & Cooper 1985)  
3.11, 3.24, 3.28  (bleak, 28-d exposure, Bengtsson et al. 1986)  
Sorption Partition Coefficient, log $K_{\text{OC}}$:  
4.44  (calculated-$K_{\text{ow}}$, Muir 1984)  
3.67  (estimated from solubility, Boethling & Cooper 1985)

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

- **Volatilization:**
- **Photolysis:**
- **Oxidation:**
- **Hydrolysis:**
  - Biodegradation: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28–48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

**Biotransformation:**

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

Half-Lives in the Environment:

**Air:**
- Surface water: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28–48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

**Groundwater:**

**Sediment:**

**Soil:**

**Biota:** eliminated $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).
15.1.4.2 Triaryl/alkyl phosphates

15.1.4.2.1 Dibutyl phenyl phosphate (DBPP)

Common Name: Dibutyl phenyl phosphate
Synonym: DBPP
Chemical Name:
CAS Registry No: 2528-26-1
Molecular Formula: \( \text{C}_4\text{H}_9\text{O}_4\text{P} \) \((\text{C}_4\text{H}_9)_2\text{C}_6\text{H}_5\text{O}_4\text{P}\)
Molecular Weight: 286.303
Melting Point (°C):
Boiling Point (°C):
- 200/20 mmHg (Muir 1984)
- 155/2 mmHg, 155/1 mmHg (quoted, Boethling & Cooper 1985)
Density (g/cm³):
- 0.84, 0.307 (estimated from boiling points, Boethling & Cooper 1985)
Molar Volume (cm³/mol):
- Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
- Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
- Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), \( F \):
Water Solubility (g/m³ or mg/L at 25°C):
- 96 (shake flask-GC, Saeger et al. 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):
- 66.7 (200°C, Muir 1984)
- 0.084, 0.0307 (estimated from boiling points, Boethling & Cooper 1985)
- 0.253, 0.089 (estimated-P/C, Boethling & Cooper 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C):
- 3.23 (RP-HPTLC-k' correlation, Renberg et al. 1980)
Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
- 4.27 (shake flask-concn ratio, Saeger et al. 1979)
- 3.23 (RP-HPTLC-k' correlation, Renberg et al. 1980)
Bioconcentration Factor, \( \log K_{\text{BCF}} \):
- 2.43 (calculated, Saeger et al. 1979)
- 3.04 (calculated-K_{\text{OW}}, Boethling & Cooper 1985)
Sorption Partition Coefficient, \( \log K_{\text{OC}} \):
- 3.70 (calculated-K_{\text{OW}}, Muir 1984)
- 2.56 (soil, estimated from solubility, Boethling & Cooper 1985)
Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{\frac{1}{2}} \):
Volatilization: \( t_{\frac{1}{2}} = 0.4 \) d (calculated, Muir 1984)
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

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

Half-Lives in the Environment:

Air:
Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
volatilization $t_{1/2} \approx 0.4$ d from 1 m deep water (Muir 1984).

Groundwater:

Sediment:
Soil:

Biota:
15.1.4.2.2  2-Ethylhexyl diphenyl phosphate (EHDP)

Common Name: 2-Ethylhexyl diphenyl phosphate
Synonym: EHDP
Chemical Name:
CAS Registry No: 1241-94-7
Molecular Formula: C_{20}H_{27}O_4P, C_{8}H_{17}(C_6H_5)_2O_4P
Molecular Weight: 362.399
Melting Point (°C):
-80 (Muir 1984)
Boiling Point (°C):
181/0.6 mmHg (Wightman & Malaiyandi 1983)
239/1 mmHg (Muir 1984)
150/0.2 mmHg, 375/760 mmHg, 230/5 mmHg (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
1.9 (shake flask-GC, Saeger et al. 1979)
Vapor Pressure (Pa at 25°C):
4.0 × 10⁻³, 3.47 × 10⁻³, 1.87 × 10⁻³ (estimated from reported boiling points, Boethling & Cooper 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C):
1.60 (calculated-P/C, Muir 1982, 1984)
0.77, 0.648, 0.345 (calculated-P/C, Boethling & Cooper 1985)
Octanol/Water Partition Coefficient, log K_{ow}:
5.73 (shake flask-concn ratio, Saeger et al. 1979)
5.00 (RP-HPLC-k’ correlation, Renberg et al. 1980)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
3.20 (calculated, Saeger et al. 1979)
3.17, 3.06; 3.12 (rainbow trout: calculated from rate constant ratio k_1/k_2 for exposure concn 5 and 50 µg/L; mean, Muir & Grift 1981)
3.52 (calculated-K_{ow}, Muir & Grift 1981)
4.11 (calculated-K_{ow}, Boethling & Cooper 1985)
Sorption Partition Coefficient, log K_{oc}:
4.49 (calculated-K_{ow}, Muir 1984)
3.49 (estimated from solubility, Boethling & Cooper 1985)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volutilization: half-life for 1 m deep water was estimated to be 7 d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981).

Biotransformation:

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

$k_1 = 48.5$ h$^{-1}$, 33.0 h$^{-1}$ (rainbow trout, exposure concn 5, 50 µg/L, Muir & Grift 1981)

$k_2 = 0.0298$ h$^{-1}$, 0.0294 h$^{-1}$ (rainbow trout, exposure concn 5, 50 µg/L, Muir & Grift 1981)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981);

volatilization $t_{1/2} \sim 7$ d for 1 m deep water (estimated, Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:
15.1.4.2.3 Isodecyl diphenyl phosphate (IDDP)

![Chemical Structure](image)

Common Name: Isodecyl diphenyl phosphate
Synonym: IDDP
Chemical Name:
CAS Registry No: 29761-21-5
Molecular Formula: C_{22}H_{31}O_4P, C_{10}H_{21}(C_6H_5)_2O_4P
Molecular Weight: 390.452
Melting Point (°C):
< –50 (Muir 1984)
Boiling Point (°C):
245/10 mmHg (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Boiling Point (°C):
245/10 mmHg (Boethling & Cooper 1985)
Molar Volume (cm³/mol):
Enthalpy of Fusion, △H_{fus} (kJ/mol):
Entropy of Fusion, △S_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming △S_{fus} = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.75 (room temp, shake flask-GC, Saeger et al. 1979)
0.80 (Boethling & Cooper 1985)
Vapor Pressure (Pa at 25°C):
< 13.33, 66.7 (100, 150°C, Muir 1984)
2.133 × 10⁻³ (estimated from boiling point, Boethling & Cooper 1985)
Henry’s Law Constant (Pa·m³/mol at 25°C):
12.97 (calculated-P/C, Muir 1984)
1.013 (calculated-P/C, Boethling & Cooper 1985)
Octanol/Water Partition Coefficient, log K_{OW}:
5.44 (shake flask-concn ratio, Saeger et al. 1979)
3.31, 5.72; 5.42 (RP-HPTLC-k’ correlation; mean, Renberg et al. 1980)
5.70 (quoted measured value, Boethling & Cooper 1985)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
3.04 (calculated, Saeger et al. 1979)
3.88 (estimated from solubility, Boethling & Cooper 1985)
Sorption Partition Coefficient, log K_{OC}:
4.33 (calculated-K_{OW}, Muir 1984)
3.69 (soil, estimated from solubility, Boethling & Cooper 1985)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.3$ d for 1 m deep water system (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} \sim 1.3$ d for 1 m deep water system (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:
15.1.4.3 Tributyl phosphate (TBP)

Common Name: Tributyl phosphate
Synonym: TBP, butyl phosphate
Chemical Name: tri-n-butyl phosphate
CAS Registry No: 126-73-8
Molecular Formula: C_{12}H_{27}O_{4}P; (C_{4}H_{9})_{3}O_{4}P
Molecular Weight: 266.314
Melting Point (°C):
< –80 (Dean 1985, Stephenson & Malanowski 1987)
Boiling Point (°C):
289 (Lide 2003)
Density (g/cm³):
0.972 (25°C, Dean 1992)
0.976 (Riddick et al. 1986; Budavari 1989)
Molar Volume (cm³/mol):
273.8 (Stephenson & Malanowski 1987)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
14.67 (Dean 1992)
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 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
422* (shake flask-electrometric titration, measured range 3.4–50°C, Higgins et al. 1959)
280 (shake flask-GC, Saeger et al. 1979)
390 (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):
0.89 (extrapolated, Evans et al. 1930)
0.10, 2.0 (114, 160.2°C, Riddick et al. 1986)
\log (P/kPa) = 7.7110 – 3206.5/(t/°C + 273) (Antoine eq., Riddick et al. 1986)
\log (P/kPa) = 7.7110 – 3206.5/(T/K) (Antoine eq., liquid phase, temp range 500–562 K, Stephenson & Malanowski 1987)
0.0202 (estimated from average air-borne concn, Skene & Krzymien 1995)
0.031, 0.015, 0.026, 0.030, 0.022 (extrapolated values from various reported Antoine equations, Skene & Krzymien 1995)
0.149* (gas saturation-GC, measured range 0–80°C; Skene & Krzymien 1995)
\log (P/Pa) = 8.85629 – 1690.26/(T/K – 123.431); temp range 0–80°C, (Antoine eq. derived from exptl. data, gas saturation-GC, Skene & Krzymien 1995)
0.015 (TBP in Skydrol 500B-4 hydraulic fluid, gas saturation-GC, Skene & Krzymien 1995)

Henry’s Law Constant (Pa·m³/mol at 25°C):
2513 (estimated-P/C, Muir 1984)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octanol/Water Partition Coefficient, log $K_{OW}$:</td>
<td>4.004 (shake flask-concn ratio, Saeger et al. 1979)</td>
</tr>
<tr>
<td></td>
<td>3.99 (Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>4.004, 4.01 (quoted, Muir 1984)</td>
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<tr>
<td>Bioconcentration Factor, log BCF:</td>
<td>2.28 (calculated, Saeger et al. 1979)</td>
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<tr>
<td></td>
<td>1.49–1.54 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>0.78–1.04 (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>0.602–1.43 (killifish, static water system, Sasaki et al. 1982)</td>
</tr>
<tr>
<td></td>
<td>1.20–1.43 (killifish, 4–38 d exposure, continuous flow water system, Sasaki et al. 1982)</td>
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<td>Sorption Partition Coefficient, log $K_{OC}$:</td>
<td>3.56 (calculated-$K_{OW}$, Muir 1984)</td>
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<td>Environmental Fate Rate Constants, k, or Half-Lives, $t_\frac{1}{2}$:</td>
<td>Volatilization: $t_\frac{1}{2} = 0.4$ d for 1 m deep water system (calculated, Muir 1984).</td>
</tr>
<tr>
<td></td>
<td>Photolysis:</td>
</tr>
<tr>
<td></td>
<td>Oxidation:</td>
</tr>
<tr>
<td></td>
<td>Hydrolysis:</td>
</tr>
<tr>
<td></td>
<td>Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_\frac{1}{2} &lt; 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).</td>
</tr>
<tr>
<td></td>
<td>Biotransformation:</td>
</tr>
<tr>
<td></td>
<td>Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:</td>
</tr>
<tr>
<td>Half-Lives in the Environment:</td>
<td>Air:</td>
</tr>
<tr>
<td></td>
<td>Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_\frac{1}{2} &lt; 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979); hydrolysis $t_\frac{1}{2} \sim 1$ yr for trialkyl phosphates (Wolfe 1980); $t_\frac{1}{2} = 58$ h in the water containing killifish and more than 100 h for goldfish (Sasaki et al. 1981) volatilization $t_\frac{1}{2} \sim 0.4$ d from 1 m deep water (estimated, Muir 1984).</td>
</tr>
<tr>
<td></td>
<td>Groundwater:</td>
</tr>
<tr>
<td></td>
<td>Sediment:</td>
</tr>
<tr>
<td></td>
<td>Soil:</td>
</tr>
<tr>
<td></td>
<td>Biota:</td>
</tr>
</tbody>
</table>
### TABLE 15.1.4.3.1.1
Reported aqueous solubilities and vapor pressures of tributyl phosphate at various temperatures and the coefficients for the vapor pressure equations

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

<table>
<thead>
<tr>
<th>Temp. (°C)</th>
<th>Higgins et al. 1959</th>
<th>Skene &amp; Krzymien 1995</th>
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<tr>
<td></td>
<td>Aqueous solubility</td>
<td>Vapor pressure</td>
</tr>
<tr>
<td></td>
<td>S/g·m(^{-3})</td>
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<tr>
<td></td>
<td>shake flask-titration</td>
<td>gas saturation-GC</td>
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<tr>
<td>3.4</td>
<td>1075</td>
<td>0</td>
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<tr>
<td>4.0</td>
<td>1012</td>
<td>5</td>
</tr>
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<td>5.0</td>
<td>957</td>
<td>15</td>
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<td>13.0</td>
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</tr>
</tbody>
</table>

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FIGURE 15.1.4.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tributyl phosphate.

FIGURE 15.1.4.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for tributyl phosphate.
15.1.4.3.2  Tris(2-ethylhexyl) phosphate (TEHP)

Common Name: Tris(2-ethylhexyl) phosphate
Synonym: TEHP
Chemical Name:
CAS Registry No: 78-42-2
Molecular Formula: C_{24}H_{51}O_4P, (C_{8}H_{17})_3O_4P
Molecular Weight: 434.633
Melting Point (°C):
Boiling Point (°C):
    215°C/4 mmHg (Aldrich Catalog 1989–99)
Density (g/cm³ at 20°C): 0.924 (Aldrich catalog 1998–99)
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
    < 1000  (room temp, shake flask-GC, Saeger et al. 1979)
    600    (practical grade, shake flask-nephelometry, Hollifield 1979)
Vapor Pressure (Pa at 25°C):
    log (P/mmHg) = 12.85 – 5812/(T/K); exptl. data presented in graph and Antoine eq. (effusion, Small et al. 1948)
    (See figure at the end of this section.)
    1.10 × 10⁻⁵ (liquid P_l, GC-RT correlation, Hinckley et al. 1990)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
    4.23  (shake flask-concn ratio, Saeger et al. 1979)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
    2.40  (calculated, Saeger et al. 1979)
Sorption Partition Coefficient, log K_{oc}:
    3.68  (soil, calculated-K_{ow}, Muir 1984)
Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:
Volatileization:
    Photoysis:
    Oxidation:
    Hydrolysis:
    Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).
    Biotransformation:
Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:

**Air:**
Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

**Groundwater:**

**Sediment:**

**Soil:**

**Biota:**

**FIGURE 15.1.4.3.2.1** Logarithm of vapor pressure versus reciprocal temperature for tris(2-ethylhexyl) phosphate.

**FIGURE 15.1.4.3.2.1** Logarithm of vapor pressure versus reciprocal temperature for tris(2-ethylhexyl) phosphate.
### 15.1.4.4 Trihaloalkyl phosphates

15.1.4.4.1 Tris(2-chloroethyl) phosphate (TCEP)

![Chemical Structure](image)

Common Name: Tris(2-chloroethyl) phosphate  
Synonym: TCEP  
Chemical Name:  
CAS Registry No: 115-96-8  
Molecular Formula: C₆H₁₂Cl₃O₄P, (C₂H₄Cl)₃O₄P  
Molecular Weight: 285.490  
Melting Point (°C): –55

<table>
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<tr>
<td>Boiling Point (°C)</td>
<td>214/25 mmHg (Muir 1984)</td>
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<tr>
<td></td>
<td>330 (Stephenson &amp; Malanowski 1987; Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>1.390 (Aldrich catalog 1989–99)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>205.4 (20°C, Stephenson &amp; Malanowski 1987)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔH_{fus} (kJ/mol)</td>
<td>8.23 (interpolated-Antoine eq., Stephenson &amp; Malanowski 1987)</td>
</tr>
<tr>
<td>Entropy of Fusion, ΔS_{fus} (J/mol K)</td>
<td>log (P/L/kPa) = 4.346 – 1917/(T/K) (Antoine eq., temp range: 293–546 K, Stephenson &amp; Malanowski 1987)</td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:</td>
<td>1.0</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C)</td>
<td>7000 (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>7000 (quoted, Muir 1984)</td>
</tr>
<tr>
<td>Henry’s Law Constant (Pa·m³/mol at 25°C)</td>
<td>0.00241 (calculated-P/C, Muir 1984)</td>
</tr>
<tr>
<td>Octanol/Water Partition Coefficient, log K_{ow}:</td>
<td>1.43 (shake flask, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>1.48 (quoted, Muir 1984)</td>
</tr>
<tr>
<td>Octanol/Air Partition Coefficient, log K_{oa}:</td>
<td>2.40 (calculated, Saeger et al. 1979)</td>
</tr>
<tr>
<td></td>
<td>0.34 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>–0.155, –0.046 (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)</td>
</tr>
<tr>
<td></td>
<td>0.36–1.10 (killifish, static water system, Sasaki et al. 1982)</td>
</tr>
<tr>
<td></td>
<td>0.041–1.10 (killifish, continuous flow water system, Sasaki et al. 1982)</td>
</tr>
<tr>
<td>Sorption Partition Coefficient, log K_{oc}:</td>
<td>2.18 (calculated-K_{owc}, Muir 1984)</td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, $k_i$, or Half-Lives, $t_{1/2}$:

- **Volatilization**: $t_{1/2} \approx 536$ d from 1 m deep water system (estimated, Muir 1984).
- **Photolysis**: 
- **Oxidation**: 
- **Hydrolysis**: 
- **Biodegradation**: 
- **Biotransformation**: 

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

- biological $t_{1/2} = 1.65$ h and elimination $t_{1/2} = 0.7$ h for killifish (Sasaki et al. 1982).

Half-Lives in the Environment:

- **Air**:
- **Surface water**: first order reduction process in river water, an estimated $t_{1/2} \approx 2.3$ d in Rhine River (Zoeteman et al. 1980);
  - volatilization $t_{1/2}(\text{calc}) = 536$ d from 1 m deep water system (Muir 1984).
- **Groundwater**:
- **Sediment**:
- **Soil**:
- **Biota**: biological $t_{1/2} = 1.65$ h for accumulation, $t_{1/2} = 0.7$ h for elimination in killifish (Sasaki et al. 1982).
15.1.4.4.2 Tris(1,3-dichloropropyl) phosphate (TDCPP)

Common Name: Tris(1,3-dichloropropyl) phosphate
Synonym: TDCPP, TCPP, Fyrol FR-2, 1,3-dichloro-2-propanol phosphate (3:1), phosphoric acid tris(1,3-dichloro-2-propyl)ester, tris[2-chloro-1-(chloromethyl)ethyl]phosphate
Chemical Name:
Use: flame retardant
CAS Registry No: 40120-74-9
Molecular Formula: C₉H₁₅Cl₆O₄P, (C₃H₅Cl₂)₃O₄P
Molecular Weight: 430.906
Melting Point (°C):
26.7 (Muir 1984)
viscous liquid (Budavari 1989)
Boiling Point (°C):
236–237/5 mmHg (Muir 1984)
Density (g/cm³ at 20°C):
1.5022 (Budavari 1989)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.966
Water Solubility (g/m³ or mg/L at 25°C):
19.2 (Metcalf 1976)
7.0 (practical grade, shake flask-nephelometry, Hollifield 1979)
~ 100 (Budavari 1989)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
3.76 (shake flask-concn ratio, Sasaki et al. 1981)
3.74 (quoted, Muir 1984)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
1.89–2.05 (killifish, 100-h exposure, static system, Sasaki et al. 1981)
0.48–0.70 (goldfish, 90-h exposure, static system, Sasaki et al. 1981)
1.67–2.03 (killifish, static system, Sasaki et al. 1982)
1.49–1.69 (killifish, 32-d exposure, continuous flow water system, Sasaki et al. 1982)
Sorption Partition Coefficient, log K_{oc}:
3.41 (calculated-K_{ow}, Muir 1984)
Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:
Volutilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
$t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Groundwater:
Sediment:
Soil:
Biota: biological $t_{1/2} = 1.65$ h (killifish, Sasaki et al. 1982).
15.1.4.4.3  Tris(2,3-dibromopropyl) phosphate (TDBPP)

Common Name: Tris(2,3-dibromopropyl) phosphate  
Synonym: TDBPP, Tris-BP, 2,3-dibromo-1-propanol phosphate(3:1), phosphoric acid tris(2,3-dibromopropyl) ester,  
Apex 462-3, Flammex AP, Firemaster: V-T 23P, Fyrol HB 32

Chemical Name:
Use: flame retardant
CAS Registry No: 126-72-7
Molecular Formula: C₉H₁₅Br₆O₄P, (C₃H₅Br₂)₃O₄P
Molecular Weight: 697.610
Melting Point (°C):
  5.5 (Muir 1984)  
  viscous liquid (Budavari 1989)
Boiling Point (°C):
  65/0.005 mmHg (Muir 1984)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ∆H_fus (kJ/mol):
Entropy of Fusion, ∆S_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S_fus = 56 J/mol K), F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  8.0 (practical grade, shake flask-nephelometry, Hollifield 1979)
  1.60 (Muir 1984)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol at 25°C):
  0.0108 (calculated-P/C, Muir 1984)
Octanol/Water Partition Coefficient, log K_ow:
  4.98 (HPLC-RT correlation, Veith et al. 1979)
  4.39 (Muir 1984)
Octanol/Air Partition Coefficient, log K_oa:
Bioconcentration Factor, log BCF:
  0.44 (calculated-K_ow, Veith et al. 1979)
Sorption Partition Coefficient, log K_sw:
  3.76 (calculated-K_ow, Muir 1984)
Environmental Fate Rate Constants, k, or Half-Lives, t½:
  Volatilization: t½ (calc) = 1.9 d in 1 m deep water system (Muir 1984).
  Surface water: volatilization t½(calc) = 1.9 d in 1 m deep water system (Muir 1984).
# 15.2 SUMMARY TABLES AND QSPR PLOTS

## TABLE 15.2.1
Summary of physical properties of esters and phthalate esters

<table>
<thead>
<tr>
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<td><strong>Aliphatic esters:</strong></td>
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<tr>
<td>Methyl formate</td>
<td>107-31-3</td>
<td>HCO$_2$CH$_3$</td>
<td>60.052</td>
<td>–99</td>
<td>31.7</td>
<td>1</td>
<td>61.64</td>
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<tr>
<td>Ethyl formate</td>
<td>109-94-4</td>
<td>HCO$_2$C$_2$H$_5$</td>
<td>74.079</td>
<td>–79.6</td>
<td>54.4</td>
<td>1</td>
<td>80.35</td>
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<tr>
<td>Propyl formate</td>
<td>110-74-7</td>
<td>C$_3$H$_8$O$_2$</td>
<td>88.106</td>
<td>–92.9</td>
<td>80.9</td>
<td>1</td>
<td>97.30</td>
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<tr>
<td>Butyl formate</td>
<td>592-84-7</td>
<td>C$_4$H$_8$O$_2$</td>
<td>102.132</td>
<td>–91.9</td>
<td>106.1</td>
<td>1</td>
<td>110.8</td>
</tr>
<tr>
<td>Isobutyl formate</td>
<td>542-55-2</td>
<td>C$_5$H$_8$O$_2$</td>
<td>102.132</td>
<td>–95.8</td>
<td>98.2</td>
<td>1</td>
<td>133</td>
</tr>
<tr>
<td>Methyl acetate</td>
<td>79-05-9</td>
<td>(CH$_3$)$_2$CO</td>
<td>74.079</td>
<td>–98.25</td>
<td>56.87</td>
<td>1</td>
<td>79.30</td>
</tr>
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<td>Vinyl acetate</td>
<td>108-05-4</td>
<td>C$_4$H$_8$O$_2$</td>
<td>86.09</td>
<td>–93.2</td>
<td>72.8</td>
<td>1</td>
<td>92.40</td>
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<td>Allyl acetate</td>
<td>591-87-7</td>
<td>C$_4$H$_8$O$_2$</td>
<td>100.117</td>
<td>–83.8</td>
<td>77.11</td>
<td>1</td>
<td>97.83</td>
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<td>Ethyl acetate</td>
<td>141-78-6</td>
<td>C$_5$H$_10$O$_2$</td>
<td>102.132</td>
<td>–93</td>
<td>101.54</td>
<td>1</td>
<td>115.04</td>
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<td>Propyl acetate</td>
<td>109-60-4</td>
<td>C$_5$H$_10$O$_2$</td>
<td>116.158</td>
<td>–78</td>
<td>126.1</td>
<td>1</td>
<td>132.54</td>
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<tr>
<td>Butyl acetate</td>
<td>123-86-4</td>
<td>C$_6$H$_12$O$_2$</td>
<td>116.158</td>
<td>–98.8</td>
<td>116.5</td>
<td>1</td>
<td>155.2</td>
</tr>
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<td>Isobutyl acetate</td>
<td>110-19-0</td>
<td>C$_7$H$_14$O$_2$</td>
<td>130.185</td>
<td>–70.8</td>
<td>149.2</td>
<td>1</td>
<td>148.51</td>
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<td>Penty acetate</td>
<td>628-63-7</td>
<td>C$_7$H$_14$O$_2$</td>
<td>130.185</td>
<td>–78.5</td>
<td>142.5</td>
<td>1</td>
<td>177.4</td>
</tr>
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<td>Isopentyl acetate</td>
<td>123-92-7</td>
<td>C$_8$H$_16$O$_2$</td>
<td>144.212</td>
<td>–80.9</td>
<td>171.5</td>
<td>1</td>
<td>199.6</td>
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<td>Hexyl acetate</td>
<td>142-92-7</td>
<td>C$_8$H$_16$O$_2$</td>
<td>144.212</td>
<td>–78.5</td>
<td>142.5</td>
<td>1</td>
<td>177.4</td>
</tr>
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<td>Cyclohexyl acetate</td>
<td>622-45-7</td>
<td>C$_8$H$_14$O$_2$</td>
<td>142.196</td>
<td>–83.8</td>
<td>77.11</td>
<td>1</td>
<td>97.83</td>
</tr>
<tr>
<td>2-Ethylhexyl acetate</td>
<td>103-09-3</td>
<td>C$_9$H$_18$O$_2$</td>
<td>172.265</td>
<td>–80</td>
<td>199</td>
<td>1</td>
<td>244</td>
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<td>21</td>
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### Phthalate esters:

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<th>Mw</th>
<th>Tsub</th>
<th>Tfoh</th>
<th>Tfoh</th>
<th>∆S_{ fus }</th>
<th>T</th>
<th>Mw</th>
<th>T</th>
<th>Mw</th>
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<td>524.8</td>
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<td>547.0</td>
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<td>Tfoh</td>
<td>Tfoh</td>
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<td>T</td>
<td>Mw</td>
<td>T</td>
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* Assuming ∆S_{ fus } = 56 J/mol K.
### TABLE 15.2.2
Summary of selected physical-chemical properties of esters and phthalate esters at 25°C

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<td>20500</td>
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<td>10000</td>
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<td><strong>Aromatic esters:</strong></td>
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<td>Diethyl phthalate (DEP)</td>
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<td>$1.33 \times 10^{-5}$</td>
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TABLE 15.2.3
Suggested half-life classes for esters and phthalate esters in various environmental compartments at 25°C

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<td>Di-n-butyl phthalate (DBP)</td>
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<td>5</td>
<td>6</td>
<td>7</td>
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<tr>
<td>bis(2-Ethylhexyl)-phthalate (DEHP)</td>
<td>3</td>
<td>5</td>
<td>6</td>
<td>7</td>
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<tr>
<td>Butyl benzyl phthalate (BBP)</td>
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where,

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<th>Range (hours)</th>
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<td>10–30</td>
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<td>55 (~ 2 days)</td>
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<td>4</td>
<td>170 (~ 1 week)</td>
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<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>~ 5 years</td>
<td>&gt; 30,000</td>
</tr>
</tbody>
</table>
FIGURE 15.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for esters.

FIGURE 15.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for esters.
**FIGURE 15.2.3** Octanol-water partition coefficient versus Le Bas molar volume for esters.

**FIGURE 15.2.4** Henry’s law constant versus Le Bas molar volume for esters.
FIGURE 15.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for esters.
15.3 REFERENCES


CHEMFATE The Environmental Fate Database-A Computerized Database by Technical Database Services Incorporated, New York, New York.


