14 Phenolic Compounds

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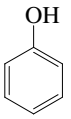
14.1 LIST OF CHEMICALS AND DATA COMPILATIONS

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: C_6H_5OH
Molecular Weight: 94.111
Melting Point (°C):
40.89 (Lide 2003)
Boiling Point (°C):
181.87 (Lide 2003)
Density (g/cm^3 at 20°C):
1.5479 (supercooled liq., Ericksen & Dobbert 1955)
1.0576 (Weast 1982)
Acid Dissociation Constant, pK_a:
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)
9.92 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Varhaníčková et al. 1995)
10.05 (Saarikoski 1982; Saarikoski & Viluksela 1982)
9.90 (UV absorption, Hoigné & Bader 1983; Scully & Hoigné 1987)
9.99 (Dean 1985; Schultz & Cajina-Quezada 1987; Hersey et al. 1989)
10.93 (Miyake et al. 1987)
10.12 (UV spectrophotometry, Nendza & Seydel 1988)
Molar Volume (cm^3/mol):
89.0 (20°C, calculated-density)
103.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (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/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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)

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88360 (shake flask-UV at pH 5.1, Blackman et al. 1955)
79000* (20°C, synthetic method/shake flask-optical, measured range 0–68.3°C, Ericksen & Dobbert 1955)
80000 (20°C, Mulley & Metcalf 1966)
78000 (shake flask-spectrophotometry, Roberts et al. 1977)
79750 (shake flask-GC, Kraij & Sincic 1980)
76514 (generator column-HPLC, Wasik et al. 1981)
150580 (20°C, shake flask-UV, Hashimoto et al. 1984)
87000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
84045* (shake flask-conductimetry, measured range 15.1–35°C, Achard et al. 1996)
94100* (25.35°C, shake flask-optical method, measured range 298.5–336.7 K, Jaoui et al. 1999)
83119* (23.15°C, shake flask-optical method, measured range 292.5–333.6 K, Jaoui et al. 2002)
ln [S/(mol kg^{-1})] = 7.3013 – 853.62/(T/K); temp range 288–313 K (eq.-I derived using reported exptl. data, Jaoui et al. 2002)
ln [S/(mol kg^{-1})] = 10.731 – 1931.7/(T/K); temp range 313–332 K (eq.-II derived using reported exptl. data, Jaoui 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):
133.3* (44.8 °C, static method-manometer, measured range 44.8–181.4 °C, Kahlbaum 1898)
28531* (141.1 °C, mercury manometer, measured range 141.1–181.1 °C, Goldblum et al. 1947)
log (P/mmHg) = –2510/(T/K) + 8.395; temp range: 141.1–181.1°C (Hg manometer, Goldblum et al. 1947)
55.54* (extrapolated-regression of tabulated data, temp range 40.1–181.9°C, Stull 1947)
7605* (107.15 °C, ebulliometry, measured range 107.15–181.75 °C, Dreisbach & Shrader 1949)
1333* (70.50 °C, ebulliometry, measured range 70.50–181.7 °C, Vonterres et al. 1955)
70.75 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.57893 – 1817.0/(205.0 + t/°C), temp range: 93–240°C, (Antoine eq. for liquid state, Dreisbach 1955)
44.26* (24.85°C, gas saturation and diaphragm manometer measurements, measured range 0–37.5°C, Biddiscombe & Martin 1958)
45.71 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
log (P/mmHg) = 11.5638 – 3586.36/(t/°C + 273); temp range 9–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
log (P_L/mmHg) = 7.13457 – 1615.072/(t/°C + 174.569); temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
45.07 (interpolated- Antoine eq., Andon et al. 1960)
70.70 (20°C, supercooled liq., Andon et al. 1960)
83.95 (extrapolated supercooled liquid value, Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 11891.5/(T/K)] + 8.513843; temp range 40.1–418.7°C (Antoine eq., Weast 1972–73)
47.01 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.13301 – 1516.79/(174.954 + t/°C); temp range 107–182°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
26.66, 133.3 (20°C, 40°C, Verschueren 1977, 1983)
16.27 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 454.610/(T/K)] × 10^{1.00375 – 8.88757 × 10^{-4}·(T/K) + 6.83750 × 10^{-7}·$(T/K)^2$}; temp range: 323.205–694.25 K, (Cox eq., Chao et al. 1983)
46.91, 54.74 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.25543 – 1515.182/(174.182 + t/°C); temp range 107–181.75°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/kPa) = 6.70346 – 1793.899/(200.218 + t/°C); temp range 70.5–181.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
47.00 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.1330 – 1516.79/(174.95 + t/°C); temp range 107–182°C (Antoine eq., Dean 1985, 1992)
55.00 (selected, Riddick et al. 1986)
45.7, 45.32 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

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log (P_S/kPa) = 10.6887 – 3586.36/(T/K); temp range 282–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = 10.71099 – 3594.703/(T/K); temp range 273–313 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.25947 – 1516.072/(–98.581 + T/K); temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.34757 – 1482.82/(–113.862 + T/K); temp range 455–655 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.57957 – 1710.287/(–80.273 + T/K); temp range 314–395 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.26694 – 1522.07/(–97.834 + T/K); temp range 387–456 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.30177 – 1548.368/(–94.612 + T/K); temp range 449–526 K (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)
log (P_L/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 investigation 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 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):
0.0402 (exptl., 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)
k_H/kPa = 2.69 × 10^9 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 K_{AW} = 8.701 – 5760/(T/K), temp range 20–100°C (vapor-liquid equilibrium measurements with additional literature data, Dohnal & Fenclová 1995)
0.0342* (313.24 K, derived from measured P, temp range 313.240–363.14 K, Tabai et al. 1997)
k_H/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 K_{OW}. 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)

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1.510* (20 °C, shake flask-concn ratio, measured range 10–60 °C, Korenman & Udalova 1974)
1.46, 1.61 (LC-k′ correlation, calculated-π const., Carlson et al. 1975)
1.54 (shake flask-UV, Davis et al. 1976)
1.45 (HPLC-RT correlation, Mirrlees et al. 1976)
1.48 ± 0.02 (shake flask at pH 7, Unger et al. 1978)
1.48, 1.46, 1.49, 1.51, 0.62, 2.20 (literature values, Hansch & Leo 1979)
1.46 (HPLC-k′ correlation, Butte et al. 1981; Butte et al. 1987)
1.45 (generator column-HPLC/UV, Wasik et al. 1981)
1.54 (RP-HPLC-k′ correlation, D′Amboise & Hanai 1982)
1.28, 1.54 (RP-LC-k′ correlation, calculated-fragment const. as per Rekker 1977, Hanai & Hubert 1982)
1.54 (HPLC-k′ correlation, Miyake & Terada 1982; Miyake et al. 1987)
1.62 (inter-laboratory, shake flask average, Eadsforth & Moser 1983)
1.16 (inter-laboratory, HPLC average, Eadsforth & Moser 1983)
1.49, 1.53 ± 0.09 (selected best lit. value, exptl.-ALPM, Garst 1984)
1.46, 1.55 ± 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
1.08 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.46 (RP-HPLC-RT correlation, Chin et al. 1986)
1.00, 1.42 (HPLC-k′ correlation, Eadsforth 1986)
1.46 (shake flask-CPC centrifugal partition chromatography, Berthod et al. 1988)
1.46 (RP-HPLC-capacity ratio correlation, Minick et al. 1988)
1.46 (HPLC-RT correlation, Shigeota et al. 1988)
1.52 ± 0.01 (filter chamber-UV, Hersey et al. 1989)
1.50 (recommended, Sangster 1989, 1993)
1.52, 1.58, 1.69 (CPC-RV correlation, Gluck & Martin 1990)
1.47 (shake flask-UV, Kramer & Henze 1990)
1.37 ± 0.06 (liquid-liquid extraction-flow injection-UV, Kubá 1991)
1.57 (shake flask-GC, Kishino & Kobayashi 1994)
1.46 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

4.16 (total ^{14}C in fathead minnow, mean exposure level 0.0025 $\mu g \cdot mg^{-1}$, Call et al. 1980)
4.23 (total ^{14}C in fathead minnow, mean exposure level 0.0327 $\mu g \cdot mg^{-1}$, Call et al. 1980)
4.20 (total ^{14}C in fathead minnow, mean value, Call et al. 1980)
2.20 (goldfish, rate constant ratio k_1/k_2, Nagel & Urich 1980)
0.97 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.30, 2.30, 3.34 (golden ide, algae, activated sludge, Freitag et al. 1985)
2.30 (*chlorella fusca*, Freitag et al. 1985; quoted, Howard 1989)
1.20 (algae, maximum apparent BCF, Hardy et al. 1985)
0.544 (algae, real BCF with biotransformation, Hardy et al. 1985)
3.14 (*daphnia magna*, estimated-^{14}C activity and on dry wt. basis, Dauble et al. 1986)
2.44 (*daphnia magna*, based on elimination phase, Dauble et al. 1986)
1.28 (*daphnia magna*, Dauble et al. 1986; quoted, Geyer et al. 1991)
1.24 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log K_{OC}:

1.43 (soil, Kenaga & Goring 1980)
1.48 (20°C, sorption isotherm, converted form K_{OM} organic carbon in soils, Briggs 1981)
1.15 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.57, 1.96 (silt loams, Scott et al. 1983, quoted, Howard 1989)
3.46 (untreated fine sediment, Isaacson & Frink 1984)
3.49 (untreated coarse sediment, Isaacson & Frink 1984)
1.35 (HPLC-k′ correlation, mobile phase buffered to pH 3, Hodson & Williams 1988)
2.17 (soil, calculated-K_{OW}, Howard 1989)
2.4, 2.43 (soil: quoted, calculated-MCI χ, Meylan et al. 1992)

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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 $^1\chi$, 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, C_{18} column, Hong et al. 1996)
1.32; 2.43 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
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. 1998, 1999)
1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
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, $t_{½}$:

Volatilization: estimated $t_{½}$ ~ 3.2 months for evaporation from water (Howard 1989);
$t_{½}$ = 88 d, calculated 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; quoted, Howard 1989).

Photolysis: phototransformation rate k = 0.015 h^{-1} with $t_{½}$ = 46 h in the summer (mean temp 24°C) and k = 0.0040 h^{-1} with $t_{½}$ = 173 h in the winter (mean temp 10°C) in distilled water; k = 0.018 h^{-1} with $t_{½}$ = 39 h in the summer and k = 0.0074 h^{-1} with $t_{½}$ = 94 h in the winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);
photomineralization rate k = 0.04 h^{-1} with $t_{½}$ = 16 d in the summer and k = 0.0041 h^{-1} with $t_{½}$ = 169 d in the winter in distilled water; k = 0.095 h^{-1} with $t_{½}$ = 7 d in the summer and k = 0.010 h^{-1} with $t_{½}$ = 73 d in winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);
atmospheric $t_{½}$ = 46 to 173 h, based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter; aquatic photolysis $t_{½}$ = 46 to 173 h, 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 $\lambda > 285$ nm, k = $(3.10 \pm 0.10) \times 10^{-2}$ h^{-1} in purified water (Zamy et al. 2004)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k = 1×10^4 M^{-1} s^{-1} for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{½}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
k < 2×10^2 M^{-1} s^{-1} for the reaction with singlet oxygen at 25°C with $t_{½}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
$k_{NO3} = (2.0 \pm 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at (300 ± 1) K (Carter et al. 1981)
k = 6.5×10^3 s^{-1}, dye-sensitized photooxidation first-order rate constant, second order k = $(1.3 \pm 0.2) \times 10^3$ M^{-1} s^{-1} for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 1.7–2.0 and 20–23°C (Hoigné & Bader 1983a)
$k_{NO3} = (2.10 \pm 0.50) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson et al. 1984)
$k_{NO3} = (3.64 \pm 0.14) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 294 K with reference to reaction for NO_3 radical with 2-methyl-2-butene (Atkinson et al. 1984; quoted, Atkinson 1991)
k_{OH}(exptl) = 28.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 45.5×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson et al. 1985)
k_{OH}(calc) = 36×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and k_{OH}(obs) = 28.3×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)
k = (2 to 3) × 10^6 M^{-1} s^{-1} at pH 8, 1.9×10^7 M^{-1} s^{-1} at pH 9, 4.6×10^7 M^{-1} s^{-1} at pH 9.5, 9.0×10^7 M^{-1} s^{-1} at pH 10 and 1.8×10^8 M^{-1} s^{-1} at pH 11.5 for the reaction with singlet oxygen at (19 ± 2)°C in water (Scully & Hoigné 1987)
$k_{NO3} = 3.63 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)
$k_{OH} = 26.3 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989, 1990)
$k_{NO3} = (2.59 \pm 0.52) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 300 ± 1 K with reference to reaction for NO_3 radicals with *cis*-2-butene (Atkinson 1991)

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$k = (2.6 \pm 4) \times 10^6$ M^{-1} s^{-1} for the reaction with singlet oxygen in aqueous phosphate buffer at (27 ± 1)°C (Tratynyek & Hoigné 1991)

$k_{OH} = 10.45 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{NO3} = 11.44 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (Müller & Klein 1991)

$k_{NO3} = (3.92 \pm 0.25) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K with reference to reaction for NO_3 radical with 2-methyl-2-butene; $k_{OH} = 26.5 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson et al. 1992)

k_{OH}(calc) $= 12 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (molecular orbital estimation method, Klamt 1993)

$k_{OH} = 2.6 \times 10^{-11}$ cm^3 mol^{-1} s^{-1}, and k_{OH}(aq.) $= 6.7 \times 10^9$ M^{-1} s^{-1}, the calculated atmospheric lifetime $\tau = 0.45$ d under clear sky; $\tau = 0.38$ 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: $t_{½}$ =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)

$k_B = (0.094 \pm 0.003)$ h^{-1} at feed concentration of 180 mg/L at 20°C and $k = (0.095 \pm 0.007)$ 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 $t_{½} = 20$ d in ground water; $k_B = 0.065$ d^{-1} with $t_{½} = 11$ d in Lester River water; $k_B = 0.247$ d^{-1} with $t_{½} = 3$ d in Superior harbor waters (Vaishnav & Babeu 1987)

$k_B = 0.03$ h^{-1} and $t_{½} = 28$ h for estuarine water in summer (mean temp 24°C) and $k_B = 0.011$ h^{-1} with $t_{½} = 62$ h in winter (mean temp. 10°C); $k_B = 0.4$ h^{-1} with $t_{½} = 2$ d in summer and $k_B = 0.0051$ h^{-1} with $t_{½} = 146$ 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 $t_{½} = 9$ 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)

$t_{½}$(aerobic) = 0.25 d, $t_{½}$(anaerobic) = 8.0 d in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation $k = (7.1 \pm 1.3) \times 10^{-12}$ L·organism^{-1} h^{-1} (Paris et al. 1982);

estimated bacterial transformation $k = 3 \times 10^{-6}$ mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982);

microbial transformation rate constants in pond and river samples $k = (2.0 \pm 1.5) \times 10^{-10}$ to $(4.8 \pm 3.1) \times 10^{-10}$ L $organism^{-1}$ h^{-1} at five different sites (Paris et al. 1983; quoted, Steen 1991);

degradation rate constants $k = 1.08 \times 10^{-16}$ mol $cell^{-1}$ h^{-1} from pure culture studies and $k = 0.90 \times 10^{-12}$ to 3.00×10^{-12} 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:

$k_1 = 3.15$ h^{-1}; $k_2 = 0.02$ h^{-1} (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: $t_{½} = 0.61$ d by reaction with OH radicals in air (Howard 1989);

$t_{½} = 2.28$ to 22.8 h, based on reaction with OH radical (Howard et al. 1991)

degradation $k = 0.0462$ d^{-1} corresponding to $t_{½} = 360$ h in air (Guinee & 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, NO_3 radical, respectively (Atkinson 2000).

atmospheric lifetime $\tau = 0.45$ d under clear sky and $\tau = 0.38$ d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.26$ d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: rate constant $k = (1.3 \pm 0.2) \times 10^3$ M^{-1} s^{-1} for the reaction with ozone at pH 2.0–6.0 (Hoigné & Bader 1983);

$t_{½} = 46$ h in summer, $t_{½} = 173$ h in winter in distilled water and $t_{½} = 39$ h in summer, $t_{½} = 94$ h in winter in estuarine water, based on phototransformation rate when exposed to full sunlight and microbes (Hwang et al. 1986)

$t_{½} = 43$ h in summer, $t_{½} = 118$ h in winter in poisoned estuarine water, based on photo-transformation rate and $t_{½} = 384$ h or 16 d in summer, $t_{½} = 2640$ h or 110 d in winter in poisoned estuarine water, based on photomineralization rate (Hwang et al. 1986);

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$t_{½}$ = 384 h or 16 d in summer, $t_{½}$ = 4056 h or 169 d in winter in distilled water; and $t_{½}$ = 168 h or 7 d in summer, $t_{½}$ = 1752 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);

$t_{½}$ = 2000 h in water at pH 8 and 19 ± 2°C for the reaction with singlet oxygen (Scully & Hoigné 1987);

biodegradation $t_{½}$ = 11 d in river waters and $t_{½}$ = 3 d in Superior harbor waters (Vaishnav & Babeu 1987);

complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with $t_{½}$ = 9 d in estuary river (Howard 1989);

$t_{½}$ = 77 to 3840 h in water, based on reported reaction rate constant for RO_2 radical with the phenols class, $t_{½}$ = 5.3 to 56.5 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

degradation rate constant k = 0.0217 d^{-1} corresponding to a $t_{½}$ = 766 h in water (quoted from Howard 1989, Guinee & Heijungs 1993)

$t_{½}$(aerobic) = 0.25 d, $t_{½}$(anaerobic) = 8 d in natural waters (Capel & Larson 1995)

Groundwater: biodegradation $t_{½}$ = 20 d (Vashinav & Babeu 1987);

$t_{½}$ = 12 to 168 h, based on estimated aqueous 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 $t_{½}$ = 2.70 and 3.51 h of low concentration of phenol in 2 silt loam soils (Howard 1989);

$t_{½}$ = 24 to 240 h, based on aerobic soil die-away data (Howard et al. 1991);

$t_{½}$ = 4.1 d in a slightly basic sandy loam soil containing 3.25% organic matter and $t_{½}$ = 23 d in acidic clay soil with < 1.0% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992)

degradation rate constant k = 0.227 d^{-1} corresponding to a $t_{½}$ = 73.3 h in soil (quoted from Howard 1989, Guinee & Heijungs 1993).

Biota: elimination from goldfish within 4 h (Nagel & Urich 1980);

depuration $t_{½}$(obs) = 336 h, $t_{½}$(calc) = 385 h for exposure level of 0.0025 μg mL^{-1} and $t_{½}$(obs.) = 438 h, $t_{½}$(calc) = 497 h for exposure level of 0.0375 μg mL^{-1} (Call et al. 1980);

depuration $t_{½}$(calc) = 8 to 44 min in algae (Hardy et al. 1985);

half-lives in fish $t_{½}$ < 1 d for goldfish, $t_{½}$ = 14–18 d for minnow (Niimi 1987)

TABLE 14.1.1.1.1
Reported aqueous solubilities of phenol at various temperatures

1.

Hill & Malisoff 1926		Morrison 1944		Erichsen & Dobbert 1955		Achard et al. 1996	
volumetric method		thermostatic and synthetic		shake flask-optical method		shake flake-conductivity	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20.0	83600	22.7	89300	0	73000.	15.1	76044
25.0	86600	26.9	93159	10	75000	25.0	84045
30.0	92200	32.3	98617	20	79000	35.0	93098
35.0	99100	36.0	104169	30	86000		
57.30	148700	43.7	108968	40	97000		
62.74	193500	47.7	128823	50	115000		
65.79	277700	50.5	138892	60	153000		
66.01	291300	53.5	149807	62	166000		
65.79	202100	55.8	162323	64	183000		
65.84	313500	57.8	174650	66	215000		
65.86	322300	60.9	203538	67	252000		
65.84	327900			68	316000		
				68.3	365000		

(Continued)

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TABLE 14.1.1.1.1 *(Continued)*

2.

Jaoui et al. 1999		Jaoui et al. 2002	
static visual method		static visual method*	
T/K	**S/g·m^{-3}**	**T/K**	**S/g·m^{-3}**
298.5	94100	292.5	81011
307.5	99328	296.1	82959
313.4	104556	296.3	83119
313.7	143764	300.2	86290
319.8	118149	302.7	88341
324.8	134877	305.8	90901
331.5	151606	308.4	93065
336.7	182970	313.3	97186
		315.4	100169
		322.4	114416
		326.8	124024
		331.3	134394
		333.6	139814
		some data from Achard et al. 1996, Jaoui et al. 1999	

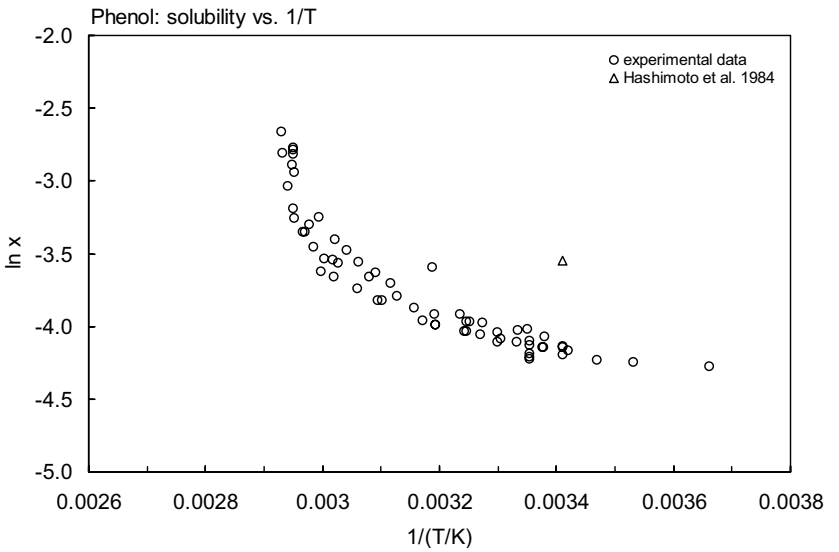

FIGURE 14.1.1.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for phenol.

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TABLE 14.1.1.1.2
Reported vapor pressures of phenol 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)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Kahlbaum 1898*		Stull 1947		Goldblum et al. 1947		Dreisbach & Shrader 1949	
static-manometer		summary of literature data		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
44.8	133.3	40.1	133.3	141.1	28531	107.15	7605
51.5	266.6	62.5	666.6	152.6	42263	113.81	10114
55.8	400.0	73.8	1333	164.4	61061	125.95	16500
59.3	533.3	86.0	2666	168.3	68661	152.37	42066
62.5	666.6	100.1	5333	173.5	80127	167.63	67661
73.5	1333.2	108.4	7999	181.0	98659	181.75	101325
85.8	2666.4	121.4	13332	140.2	27598		
93.8	3999.7	139.0	26664	145.1	32797	bp/°C	181.75
99.8	5533	160.0	53329	171.4	75194		
104.4	6661	181.9	101325	176.6	87060		
113.7	9992			181.1	98525		
120.2	13332	mp/°C	40.6				
139.0	26664			eq. 1	P/mmHg		
151.0	39997			A	8.395		
160.0	53329			B	2510		
167.0	66661						
173.0	79993						
179.0	93326						
181.4	101325						

*complete list see ref.

2.

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		solid		liquid			
70.50	1333	0	3.746	121.25	13583	40.09	173
90.20	3333	5.1	6.159	131.183	20005	50.0	345
104.2	6666	9.25	9.413	138.014	25635	60.0	655
113.0	9999	9.85	10.40	140.704	28226	70.03	1187
121.5	13332	10.4	10.47	147.204	35310	79.97	2048
132.5	19998	14.5	16.0	155.343	46139	89.99	3415
140.1	26664	18.25	22.93	156.196	47902		
147.0	33330	18.25	23.20	156.528	53130		
152.0	39997	19.6	26.66	159.799	54843		
153.0	43330	22.0	35.60	160.124	58843		
156.0	46663	24.85	44.26	163.795	60104		
160.0	53329	28.15	63.73	168.945	70154		

(Continued)

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TABLE 14.1.1.1.2 *(Continued)*

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
164.0	59995	30.5	74.39	169.991	72357		
167.0	73327	32.95	92.93	171.025	74590		
170.5	73327	35.0	108.5	172.635	78154		
173.0	79993	37.45	138.7	173.066	79148		
176.0	86659			175.767	85526		
179.0	93325	bp/°C	181.839	178.196	91590		
181.7	101325			179.878	94918		
		Antoine eq. for temp range:		180.863	98625		
		0–40°C		181.551	100497		
		eq. 1	P/mmHg	182.053	101904		
		A	11.5638				
		B	3586.36	Antoine eq. for temp range:			
		C	273	110–200°C			
				eq. 2	P/mmHg		
		ΔH_V/(kJ mol^{-1})		A	7.13457		
		at bp	47.304	B	1516.072		
		at 25°C	68.66	C	174.569		

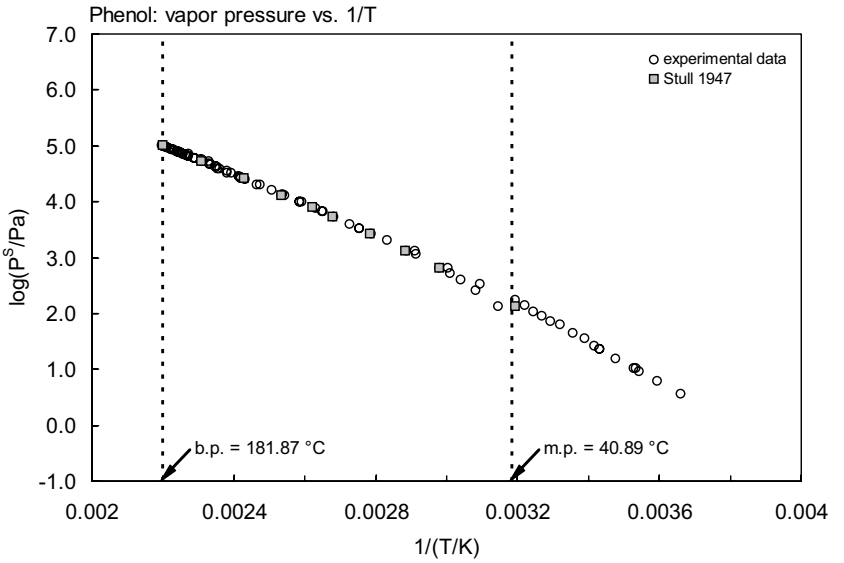

FIGURE 14.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for phenol.

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TABLE 14.1.1.1.3
Reported Henry's law constants of phenol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/atm) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4)
$\ln k_H = A - B/(T/K) - C \cdot \ln (T/K)$ (5)

$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\log H = A - B/(T/K)$ (4a)

Abd-El-Bary et al. 1986
gas stripping-GC/FID

t/°C	H/(Pa m³/mol)
–2.0	0.0072
4.0	0.0127
18.3	0.0373
27.0	0.0718
44.4	0.193*
56.3	0.437*
75.0	1.233*
90.0	2.376*

*data from literature

eq. 3	k_H/kPa
A	21.7128
B	6120.0

eq. derived included lit. data

Dohnal & Fenclová 1995
vapor-liquid equilibrium

t/°C	H/(Pa m³/mol)
4.0	0.0127*
18.3	0.0373*
27.0	0.0721*
80.3	1.552*
100.0	3.537*
75.9	1.245
88.7	2.193
98.6	3.322
25.0	0.0607#
25.0	0.0605$

#calculated from eq. 1
$calculated from eq. 3
*data from literature

eq. 1	K_{AW}
A	8.701
B	5760

enthalpy of hydration:
$\Delta H_K/(kJ\ mol^{-1}) = 47.9 \pm 0.5$
OR

eq. 3	k_H/kPa
A	21.443
B	6032

$\Delta H_K/(kJ\ mol^{-1}) = 50.2 \pm 0.4$

Tabai et al. 1997
derived from measured P

T/K	H/(Pa m³/mol)
313.24	0.0342
323.15	0.090
333.15	0.202
343.18	0.355
353.12	0.506
363.14	0.999

eq. 5	k_H/kPa
A	670.117
B	29374.5
C	94.6679

temp range 313–363 K

Harrison et al. 2002
gas stripping-UV

T/K	H/(Pa m³/mol)
284	0.0122
284.5	0.0110
289.5	0.0199
293.5	0.0262
298	0.0320
302	0.0379

eq. 4	H/(M atm⁻¹)
A	–11.6
B	–5850

Feigenbrugel et al. 2004
gas stripping-GC/MS

T/K	H/(Pa m³/mol)
278.15	0.0222
278.15	0.0299
278.20	0.0280
278.25	0.0337
283.05	0.0340
283.15	0.0456
283.15	0.0328
283.25	0.0428
283.25	0.0404
288.15	0.0590
288.15	0.0928
288.25	0.0560
293.15	0.1166
293.15	0.169
293.15	0.1093
293.15	0.1065
293.25	0.0960
293.25	0.1071
298.15	0.0904
298.15	0.2022
298.15	0.1375

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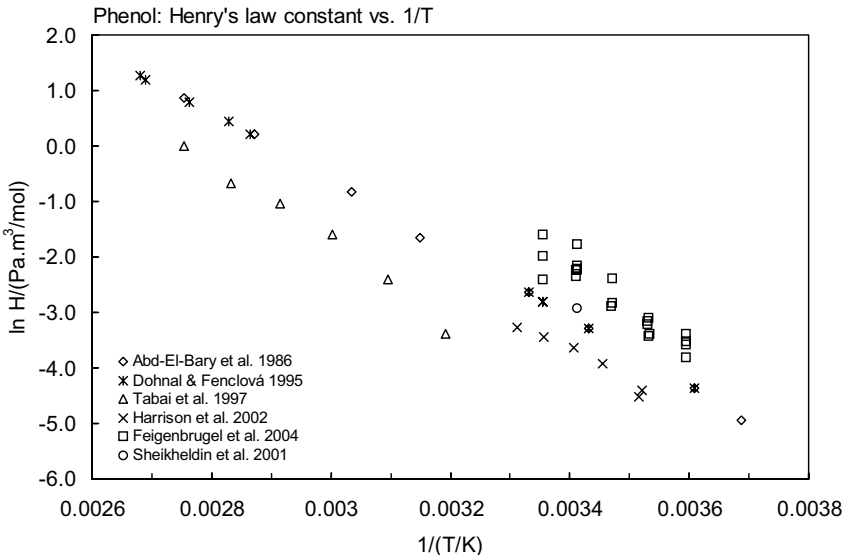

FIGURE 14.1.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for phenol.

TABLE 14.1.1.1.4
Reported octanol-water partition coefficients of phenol at various temperatures

Korenman & Udalova 1974	
shake flask-concn ratio	
t/°C	**log K_{OW}**
10	1.531
20	1.510
30	1.461
40	1.433
50	1.396
60	1.369
log K_{OW} = A – B/(T/K)	
A	0.4479
B	–305.877

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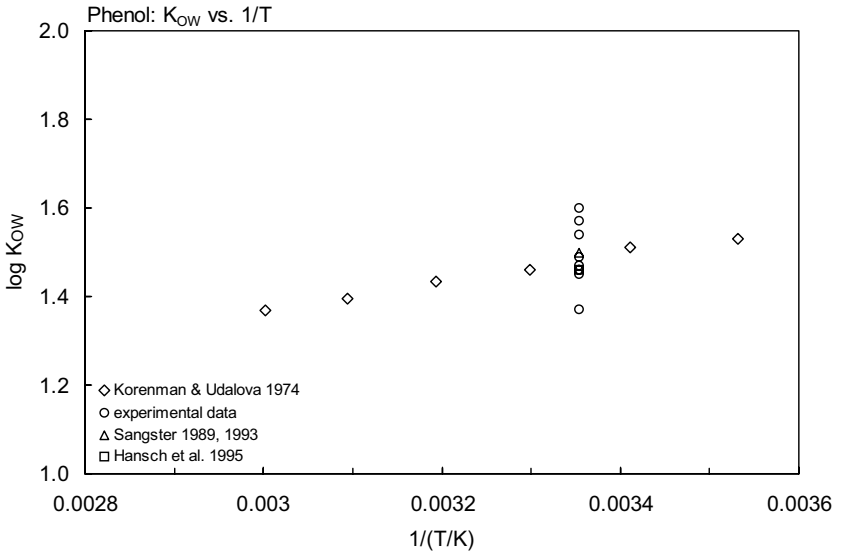

FIGURE 14.1.1.1.4 Logarithm of K_{OW} versus reciprocal temperature for phenol.

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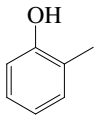
14.1.1.2 *o*-Cresol



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: C_7H_8O, $C_6H_4(CH_3)OH$
Molecular Weight: 108.138
Melting Point (°C):
31.03 (Lide 2003)
Boiling Point (°C):
191.04 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0273 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
10.28 (Pearce & Simkins 1968)
10.20 (Hoigné & Bader 1983; Weast 1982–83)
10.26 (Dean 1985)
Molar Volume (cm^3/mol):
104.4 (30°C, Stephenson & Malanowski 1987)
125.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
46.94 (Biddiscombe & Martin 1958)
45.91 (at normal boiling point, Andon et al. 1960)
42.7 (Dean 1992)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
76.02 (at 25°C, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.8 (Tsonopoulos & Prausnitz 1971; Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
52.01 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.873 (mp at 31.03°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):
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)
26820* (calculated-activity coeff. γ^{∞} data, measured range 25–35°C, 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)

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log (P/mmHg) = –2520/(T/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/(203.0 + t/°C); 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) = 12.7778 – 3970.17/(t/°C + 273); temp range 0–30°C (Antoine eq. gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
log (P/mmHg) = 7.07055 – 1542.299/(t/°C + 177.110); temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
log (P/mmHg) = [–0.2185 × 12487.3/(T/K)] + 8.79055; temp range 38.2–190.8°C (Antoine eq., Weast 1972–73)
30.7 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 6.91172 – 1435.503/(165.158 + t/°C); temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
32.0 (Verschueren 1977, 1983)
38.32 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 463.986/(T/K)] × 10^{1.01555 – 9.95980 × 10^{-4}·(T/K) + 7.92834 × 10^{-7}·$(T/K)^2$}; temp range 313.20–697.65 K (Cox eq., Chao et al. 1983)
30.3, 22.5 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.02377 – 1427.165/(164.218 + t/°C); temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/kPa) = 5.82809 – 1299.971/(148.886 + t/°C); 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/mmHg) = 6.9117 – 1435.5/(165.16 + t/°C); temp range 120–191°C (Antoine eq., Dean 1985, 1992)
37.70 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.68858 – 3909.409/(T/K); temp range 273–303 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.19545 – 1542.299/(–96.04 + T/K); temp range 383–473 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.47616 – 1714.489/(–79.841 + T/K); temp range 304–409 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.19561 – 1543.097/(–95.902 + T/K); temp range 399–470 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.24893 – 1584.403/(–90.794 + T/K); temp range 463–526 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.82237 – 2134.352/(–19.536 + T/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/K) – 32.60231·log (T/K) + 1.24267 × 10^{-2}·(T/K); temp interval of investigation: 412–467 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
log(P/mmHg) = 89.4591 – 6.0489 × 10^3/(T/K) – 29.481·log(T/K) + 1.0936 × 10^{-4}·(T/K) + 1.9933 × 10^{-12}·$(T/K)^2$; temp range 304–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/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)

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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_{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_{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_{OW}, Lyman et al. 1982; quoted, Howard 1989)
1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log K_{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_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = 3.41 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 300 ± 1 K (relative rate method with reference 2-methyl-2-butene Perry et al. 1977; Atkinson et al. 1979)
$k_{NO3} = (12 \pm 2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 300 ± 1 K (relative rate method with reference to with 2-methyl-2-butene Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)
$k < 2 \times 10^2$ M^{-1} 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)
$k_{OH} = 20 \times 10^9$ M^{-1} s^{-1} at 25°C with $t_{½}$ = 0.3 d (Hendry & Kenley 1979; quoted, Mill 1982)
$k_{NO3} = (13.9 \pm 2.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 300 ± 1 K (relative rate method with reference to the reaction of NO_3 radical with 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)
photooxidation $t_{½}$ = 66–3480 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)
$k_{O3} = (2.55 \pm 0.39) \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K; calculated tropospheric lifetimes of 45 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)
$k_{OH} = 2 \times 10^8$ M^{-1} s^{-1} with half-life of 0.3 d in the atmosphere (Mill 1982)
$k_{OH} = 2.0 \times 10^{13}$ cm^3 mol^{-1} s^{-1} at 300 K (Lyman et al. 1982)
$k = (1.2 \pm 0.3) \times 10^4$ M^{-1} s^{-1} for the reaction with ozone in water at pH 1.5–2.0 (Hoigné & Bader 1983b)

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$k_{OH} = 4.1 \times 10^{-11}$ cm³·molecule^{-1} s^{-1} at 298 K, $k_{NO3} = 1 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{NO3} = (1.20 \pm 0.34) \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 296 ± 2 K (Atkinson et al. 1984)

$k_{NO3} = (15.6 \pm 1.7) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} with reference to the reaction of NO_3 radical with *m*-cresol at (298 ± 1) K (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{NO3} = 22 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} with 2.4×10^8 NO_3 radical/cm³ at room temp. and a loss rate of 450 d^{-1} with $t_{½}$ = 1.6–16 h (Atkinson et al. 1984, 1985; quoted, Atkinson 1985)

$k_{OH} = 40 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} for the vapor-phase reaction with 5×10^5 hydroxyl radical/cm³ at room temp. and a loss rate of 1.7 d^{-1} (Atkinson 1985; quoted, Howard et al. 1991)

k_{OH}(exptl) = 37×10^{-12} cm³ molecule^{-1} s^{-1}, and k_{OH}(calc) = 44.8×10^{-12} cm³ molecule^{-1} s^{-1} at room temp. (Atkinson 1985)

k_{OH}(exptl) = 40×10^{-12} cm³ molecule^{-1} s^{-1}, k_{OH}(calc) = 44×10^{-12} cm³ molecule^{-1} s^{-1} at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{OH} = 4.2 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

$k_{NO3} = (13.7 \pm 0.9) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at (296 ± 2) K, and $k_{OH} = 42 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} for at room temp. (Atkinson et al. 1992)

k_{OH}(calc) = 30.36×10^{-12} cm³ molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

$k_{OH} = 4.9 \times 10^{-11}$ cm³ mol^{-1} s^{-1}, and k_{OH}(aq.) = 1.1×10^{-10} M^{-1} s^{-1}, the calculated atmospheric lifetime τ = 0.24 d under clear sky; τ = 0.22 d under cloudy conditions at 298 K, reduced to 0.17 d due the average temperature of tropospheric clouds at 283 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)

$t_{½}$ = 2 d at 20°C and 7 d at 4°C in river water (Ludzack & Ettinger 1960; quoted, Howard 1989)

completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation k = 54.0 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)

$t_{½}$(aq. aerobic) = 24–168 h, based on unacclimated aerobic screening test data (Takemoto et al. 1981; Urushigawa et al. 1983; quoted, selected, Howard et al. 1991)

$t_{½}$(aq. anaerobic) = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

k(exptl.) = 0.0679 h^{-1} compared to group contribution method predicted k(calc) = 0.0728 h^{-1} (nonlinear) and k = 0.0567 h^{-1} (linear) (Tabak & Govind 1993)

$t_{½}$(aerobic) = 2 d, $t_{½}$(anaerobic) = 15 d in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation k = $(2.7 \pm 1.3) \times 10^{-10}$ L·organism^{-1}·h^{-1} (Paris et al. 1983; quoted, Steen 1991).

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

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 1.6–16 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 × 10–^{4} min^{-1} in outdoor Teflon chambers in the dark (Grosjean 1985);

photodegradation $t_{½}$ ~ 9.6 h in air, based on measured rate constant for the reaction with photochemically generated hydroxyl radicals (quoted, Howard 1989);

atmospheric transformation lifetime τ < 1 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 τ = 0.24 d under clear sky and τ = 0.22 d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to τ = 0.19 d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: photooxidation $t_{½}$ = 66–3480 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 = $(1.2 \pm 0.3) \times 10^4$ M^{-1} s^{-1} for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983)

$t_{½}$(aerobic) = 2 d, $t_{½}$(anaerobic) = 15 d in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{½}$ ~0.01 yr for cresols at Noordwijk (Zoeteman et al. 1981).

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Sediment:

Soil: $t_{½}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{½}$ = 5.1 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
35.3	30100	0	22000	25	26820
50.2	32200	20	25000	30	28470
61.7	34700	40	28000	35	30810
70.6	37500	60	32000	75.9	42608
77.7	41000	80	38000	88.7	48061
84.6	45100	100	48000	98.5	52241
130.6	65200	120	67000	100	53640
148.7	104600	130	82000		
158.7	193600	140	102000		
161.7	300600	150	136000		
162.8	408900	160	202000		
160.0	501400	162	228000		
157.7	598000	164	275000		
145.7	693000	166	352000		
129.6	761400	166.5	400000		
87.5	823700				
56.6	845800				
33.6	866000				
25.6	861400				
8.3	875200				
9.1	886800				
10.2	898900				
11.1	908500				
12.9	926200				
15.3	940800				
22.3	974600				
26.9	990100				
29.9	1000000				
critical solution temp	162.8°C				
triple point	8°C				

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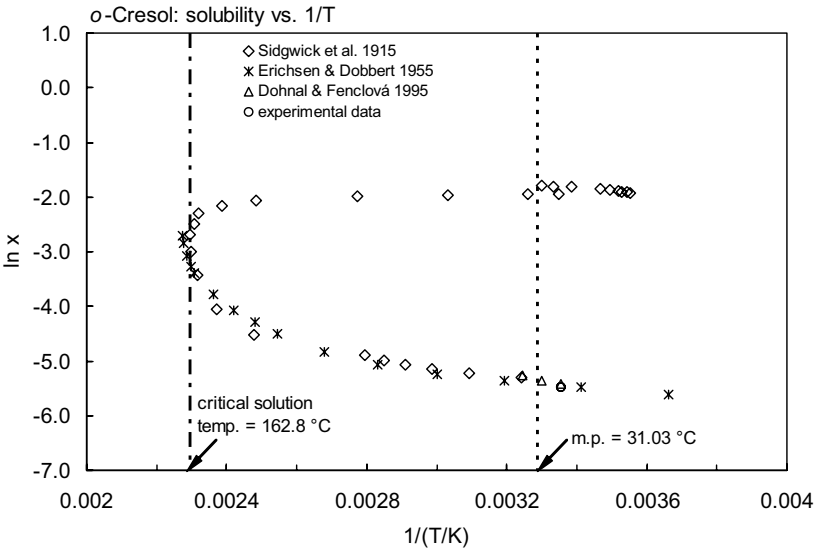

FIGURE 14.1.1.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *o*-cresol.

TABLE 14.1.1.2.2
Reported vapor pressures of *o*-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/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
							solid		liquid
38.2	133.3	142.3	23065	113.11	7605	0	2.680	138.575	20410
64.0	666.6	153.3	33731	120.22	10114	2.90	2.093	146.128	26548
76.7	1333	164.5	47729	132.63	16500	5.0	4.213	152.680	33025
90.5	2666	171.2	58529	160.17	42066	5.60	4.680	158.592	39922
105.8	5333	183.5	81993	176.14	67661	9.80	6.933	163.551	46571
115.5	7999	189.8	97859	190.95	101325	10.05	7.773	168.080	53394
127.4	13332	143.7	24265			14.85	13.20	172.002	59935
146.7	26664	166.8	51329			14.90	12.60	175.642	66563
168.4	53329	172.0	61328	bp/°C	190.95	17.40	18.27	179.039	73277
190.8	101325	179.4	73861			19.50	22.0	182.183	79956
		177.1	69194			20.0	22.40	185.185	86782
mp/°C	30.8					20.35	22.66	187.735	92934
						24.35	34.66	188.487	94810
		eq. 1	P/mmHg			25.25	37.33	189.013	96149
		A	8.308			26.65	45.20	189.455	97276
		B	2520			27.25	48.40	189.973	98613
						28.35	66.66	190.371	99650
								190.486	99953
						mp/°C	30.99	190.545	100125

(Continued)

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TABLE 14.1.1.2.2 *(Continued)*

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						bp/°C	191.003	191.046	101452
								191.135	101668
						for temp range:		191.511	102686
						0–30°C			
						eq. 2	P/mmHg		
						A	11.5638	for temp range:	
						B	3586.36	110–200°C	
						C	273	eq. 2	P/mmHg
								A	7.13457
						ΔH_v/(kJ mol^{-1})		B	1516.072
						at bp	46.94	C	174.569
						at 25°C	76.02		

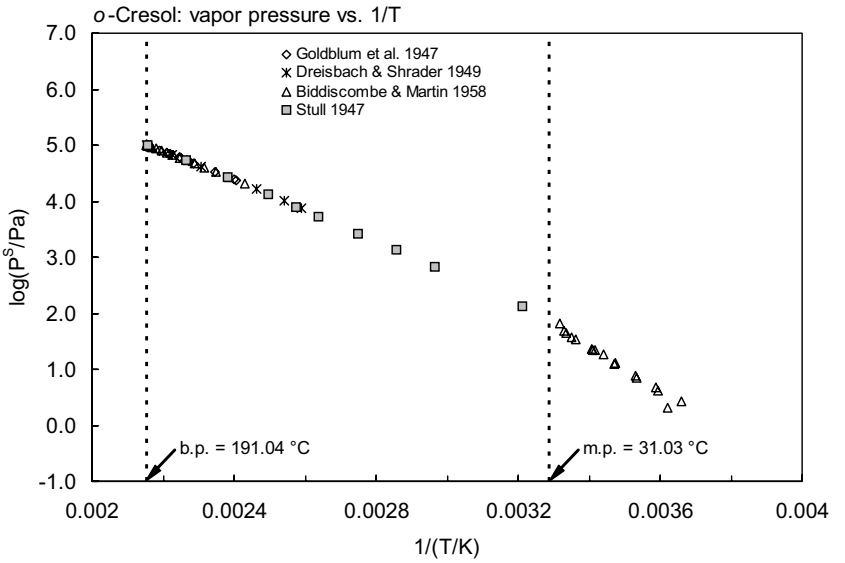

FIGURE 14.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for *o*-cresol.

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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

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/atm) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\log H = A - B/(T/K)$ (4a)

Dohnal & Fenclová 1995		Harrison et al. 2002		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-UV		gas stripping-GC/MS	
t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
25	0.176*	281	0.0224	278.25	0.0348
30	0.245*	284.5	0.0313	278.25	0.0355
35	0.341*	289.5	0.0596	278.35	0.0286
75.9	3.352	293.5	0.0650	283.15	0.0707
88.7	5.386	298	0.0965	283.15	0.0556
98.5	8.652	302	0.1165	283.25	0.0565
100	9.028			288.10	0.0842
25.0	0.1777#	eq. 4	H/(M atm^{-1})	288.15	0.1137
25.0	0.1764$	A	–15.4	288.20	0.0855
		B	–6680	293.10	0.1603
#calculated from eq. 1				293.15	0.1626
$calculated from eq. 3				293.15	0.1554
*data from literature				293.15	0.1371
				293.15	0.1883
eq. 1	K_{AW}			293.25	0.1537
A	9.091			298.15	0.2356
B	5556			298.15	0.2362
enthalpy of hydration:				293	0.1464
ΔH_K/(kJ mol^{-1}) = 46.2 ± 0.4				298	0.2390
OR					
eq. 3	k_H/kPa				
A	21.832				
B	5827				
ΔH_K/(kJ mol^{-1}) = 48.5 ± 0.4					

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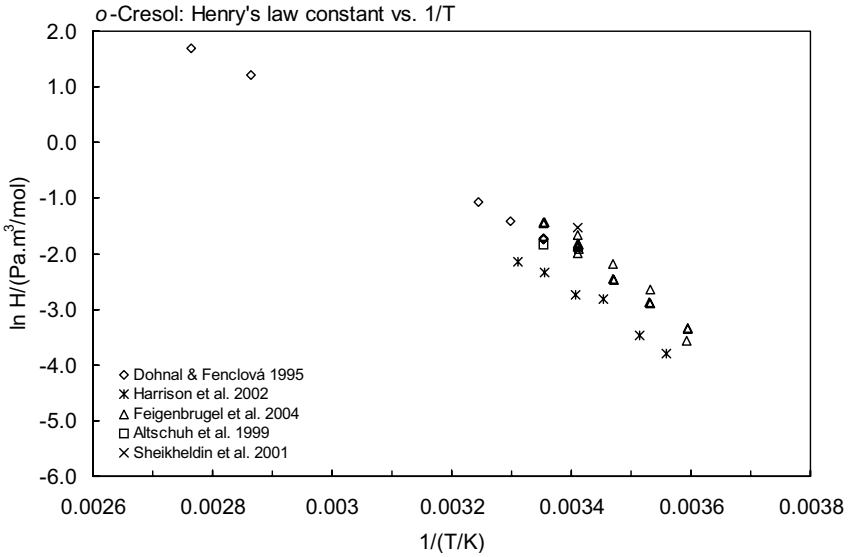

FIGURE 14.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for *o*-cresol.

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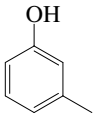
14.1.1.3 *m*-Cresol



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_7H_8O, $C_6H_4(CH_3)OH$
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, ΔH_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, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
6.53 (Tsonopoulos & Prausnitz 1971)
10.70 (Riddick et al. 1986; Dean 1992)
Entropy of Fusion, ΔS_{fus} (J/mol K):
37.53 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. 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)
24125, 23194* (24.7, 25°C, calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
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)

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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/mmHg) = –2650/(T/K) + 8.457; 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/mmHg) = 7.53165 – 1875.3/(201.0 + t/°C), 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)

19.0 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)

18.278* (24.90°C, gas saturation-diaphragm manometer, temp range 0–39°C, Biddiscombe & Martin 1958)

log (P/mmHg) = 9.9653 – 3223.45/(t/°C + 273); temp range 11–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)

log (P/mmHg) = 7.15904 – 1603.811/(t/°C + 172.646); temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; measurements, Andon et al. 1960)

log (P/mmHg) = [–0.2185 × 13483.8/(T/K)] + 9.135933; temp range 52–202.8°C (Antoine eq., Weast 1972–73)

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

log (P/mmHg) = 7.50798 – 1856.356/(199.065 + t/°C), temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

4120* (114.99°C, diaphragm gauge, measured range 114.99–216.72 °C, Nasir et al. 1980)

5.33, 16.0 (20°C, 30°C, Verschueren 1977, 1983)

36.43 (calculated-Cox eq., Chao et al. 1983)

log (P/mmHg) = [1– 475.222/(T/K)] × 10^{0.965085 – 6.89845 × 10^{-4}·(T/K) + 4.47100 × 10^{-7}·$(T/K)^2$}; temp range: 278.05–705.85 K, (Cox eq., Chao et al. 1983)

22.1, 11.9 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.62485 – 1850.362/(198.462 + t/°C); temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.28411 – 1580.594/(167.548 + t/°C); temp range 88.5–202.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

22.29 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.5080 – 1856.36/(199.07 + t/°C); temp range 150–201°C (Antoine eq., Dean 1985, 1992)

19.10 (Riddick et al. 1986)

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)

log (P_S/kPa) = 8.0462 – 2930.845/(T/K); temp range 273–285 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.28394 – 1603.811/(–100.504 + T/K); temp range 383–473 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 9.0902 – 3223.45/(T/K); temp range 284–313 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.150 – 2123.548/(–59.018 + T/K); temp range 285–416 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.28579 – 1605.855/(–100.232 + T/K); temp range 410–477 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.80987 – 1293.277/(–135.465 + T/K); temp range 471–531 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.64135 – 2069.208/(–26.534 + T/K), temp range: 523–633 K, (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)

19.70 (extrapolated-Antoine eq., Nesterova et al. 1990)

log (P/Pa) = 64.02580 – 5272.296/(T/K) – 18.84252·log (T/K) + 0.52858 × 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·log (T/K) + 1.2508 × 10^{-2}·(T/K) – 2.4317 × 0^{-12}·$(T/K)^2$; temp range 285–706 K (vapor pressure eq., Yaws 1994)

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Henry's Law Constant (Pa m^3/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)
0.1068 (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)
0.0868 (gas stripping-GC, Altschuh et al. 1999)
0.0641 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
0.0765, 0.127* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

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 $k = 0.011 \pm 0.001$ 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 NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{NO3} = (7 \pm 1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

$k_{OH} = 48 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with reference to the reaction of OH radical with 2-methyl-2-butene (Atkinson et al. 1979; Carter et al. 1981)

$k_{NO3} = (8.10 \pm 1.16) \times 10^{-12}$ $cm^3 molecule^{-1} s^{-1}$ at (300 ± 1) K with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Carter et al. 1981; quoted, Atkinson 1991)

$k_{O3} = (1.94 \pm 0.35) \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K; calculated tropospheric lifetimes of 60 d and 0.2 d due to reaction with O_3 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 RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

$k = (1.3 \pm 0.3) \times 10^4$ M^{-1} s^{-1} for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{OH} = 5.92 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

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k_{NO3} = 1×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)
k_{NO3} = $(9.20 \pm 2.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson et al. 1984)
k_{NO3} = $(15.9 \pm 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 1 K with reference to the reaction of NO_3 radical with phenol (Atkinson et al. 1984; quoted, Atkinson 1991)
k_{OH}(calc) = 93.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1} and k_{OH}(exptl) = 57×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)
k_{OH} = 6.4×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 296 K (recommended, Atkinson 1989, 1990)
k_{NO3} = $(9.74 \pm 0.74) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with reference to the reaction of NO_3 radical with 2-methyl-2-butene, and k_{OH} = 64×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson et al. 1992)
k_{OH}(calc) = 34.42×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)
k_{OH} = 5.2×10^{-11} cm^3 mol^{-1} s^{-1}, the calculated atmospheric lifetime τ = 0.22 d under clear sky; τ = 0.19 d under cloudy conditions at 298 K, reduced to 0.13 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis:
Biodegradation: $t_{½}$ = 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 $g^{-1} \cdot h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
$t_{½}$(aq. aerobic) = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
$t_{½}$(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: $t_{½}$ = 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 $t_{½}$ = 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 τ = 0.22 d under clear sky and τ = 0.19 d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to τ = 0.13 d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: $t_{½}$ = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
k = $(1.3 \pm 0.3) \times 10^4$ M^{-1} s^{-1} for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983);
photooxidation $t_{½}$ = 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, $t_{½}$ = 0.01 yr at Noordwijk (Zoeteman et al. 1981);
$t_{½}$ = 96–1176 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: $t_{½}$ = 48–696 h, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
$t_{½}$ = 11.3 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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:

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TABLE 14.1.1.3.1
Reported aqueous solubilities of *m*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Leet et al. 1987		Dohnal & Fenclová1995	
shake flask-synthetic method		shake flask-optical method		equilibrium cell-conc ratio		vapor-liquid equil.-UV	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
–0.20	22400	0	20000	20.35	23790	24.7	24125
24.7	23600	20	22000	40.05	25390	25	23194
47.0	26600	40	25000	58.45	30190	75.8	46935
61.9	30300	60	31000	77.25	37368	88.7	54615
74.5	35400	80	40000	98.15	49804	98.5	58327
87.5	42400	100	53000	119.75[a]	78100		
116.9	65900	120	88000	138.95[b]	143583		
139.4	119900	130	113000				
146.9	324000	140	156000	superscript a, at 204 kPa			
147.0	350700	142	170000	superscript b, at 366 kPa			
146.6	410600	144	189000				
140.5	612700	146	221000				
124.8	703200	147	264000				
109.3	804600	148	380000				
82.8	804600						
67.7	826000						
57.1	837000						
46.5	847900						
34.5	858500						
20.3	870500						
13.2	875800						
critical solution temp 147°C							
mp/°C	4.0						

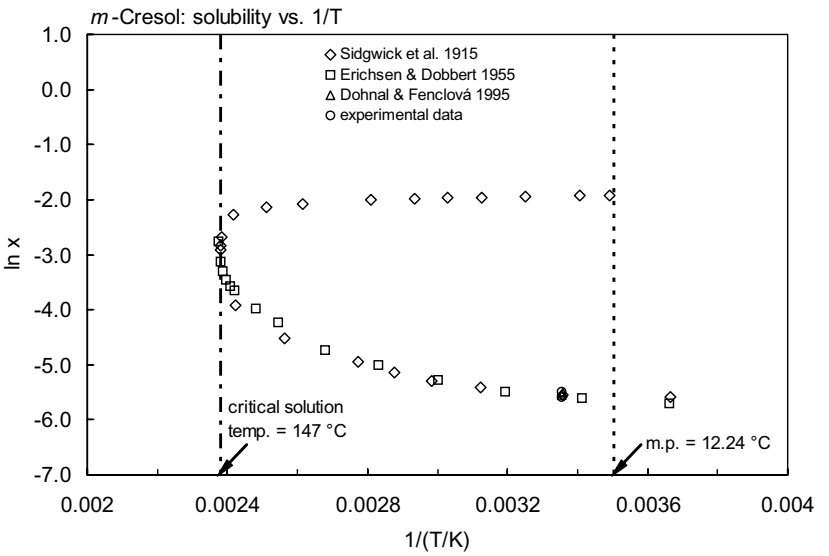

FIGURE 14.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *m*-cresol.

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TABLE 14.1.1.3.2
Reported vapor pressures of *m*-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)	$P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Goldblum et al. 1947		Vonterres et al. 1955	
summary of literature data		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
52.0	133.3	149.5	20265	85.5	1333
76.0	666.6	164.3	33464	105.2	3333
87.8	1333	172.0	42796	121.7	6666
101.4	2666	179.6	53862	131.6	9999
116.0	5333	187.4	67328	139.1	13332
125.8	7999	192.1	76927	150.0	19998
138.0	13332	196.3	86526	158.5	26664
157.3	26664	201.1	98925	163.1	33330
179.0	53329	149.6	20398	170.1	39997
202.8	101325	154.1	23731	173.0	43330
		176.4	48796	175.0	45553
mp/°C	10.8	183.4	60128	179.8	53329
		201.1	98925	183.5	66661
				189.8	73327
		eq. 1	P/mmHg	192.5	79993
		A	8.457	196.0	86659
		B	2650	198.8	93325
				202.1	101325

2.

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
			liquid				
0	2.00*	135.835	12174	114.99	4120	466.35	79960
4.90	2.933*	149.804	20418	121.25	5789	472.95	85540
7.20	4.533*	157.610	26762	127.46	7849	493.75	160600
9.15	4.40*	163.741	32816	133.4	10286	510.86	237900
11.0	5.866	169.814	39930	142.92	15223	531.35	366200
15.0	7.333	174.784	46538	156.29	25337	565.45	695500
17.65	9.866	179.331	53388	167.90	37430	588.68	1028500
19.80	11.47	182.979	59446	187.33	67950		
21.50	14.13	186.818	66415	203.4	106385	eq. 3	P/kPa
24.90	18.27	190.266	73225	216.72	149432	A	15.5337
26.95	27.73	193.424	79951			B	4594.0
29.75	30.80	196.418	86769			C	54.34
30.85	36.80	199.003	93024				

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TABLE 14.1.1.3.2 *(Continued)*

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
33.25	43.20	199.694	94754				
39.10	57.60	200.250	96156				
	*solid	200.658	97201				
		201.216	98639				
bp/°C	202.231	201.557	99550				
		202.156	101118				
Antoine eq. for temp range:		202.737	102665				
11–40°C							
eq. 2	P/mmHg	Antoine eq. for temp range					
A	9.9653	110–200°C					
B	3223.45	eq. 2	P/mmHg				
C	273	A	7.15904				
		B	1603.811				
ΔH_v/(kJ mol^{-1})		C	172.646				
at bp	49.375						
at 25°C	61.714						

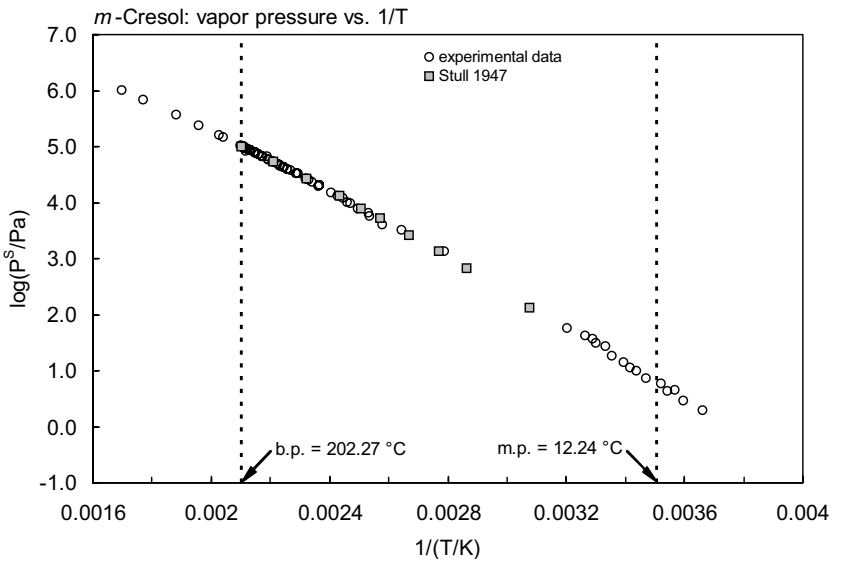

FIGURE 14.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for *m*-cresol.

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TABLE 14.1.1.3.3
Reported Henry's law constants of *m*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2)
$\ln (k_H/atm) = A - B/(T/K)$ (3)
$\ln H = A - B/(T/K)$ (4)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)
$\log K_{AW} = A - B/(T/K)$ (1a)
$\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\log H = A - B/(T/K)$ (4a)

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
24.7	0.0810*	278.15	0.0148
25.0	0.0865*	278.25	0.0192
75.9	1.683	283.15	0.0283
88.7	2.990	283.25	0.0378
98.5	4.635	283.25	0.0272
25.0	0.0848#	283.25	0.0293
25.0	0.0846$	288.15	0.0444
		288.25	0.0450
#calculated from eq. 1		293.15	0.0976
$calculated from eq. 3		293.15	0.0682
*data from literature		293.15	0.0723
		293.15	0.0786
eq. 1	K_{AW}	293.15	0.0771
A	8.909	293.15	0.0976
B	5722	293.25	0.0901
		293.15	0.0810
enthalpy of hydration:		298.15	0.1306
$\Delta H_K/(kJ\ mol^{-1}) = 47.6 \pm 0.5$		298.15	0.1252
OR		293	0.0765
eq. 3	k_H/kPa	298	0.1270
A	21.650		
B	5994		
$\Delta H_K/(kJ\ mol^{-1}) = 49.8 \pm 0.6$			

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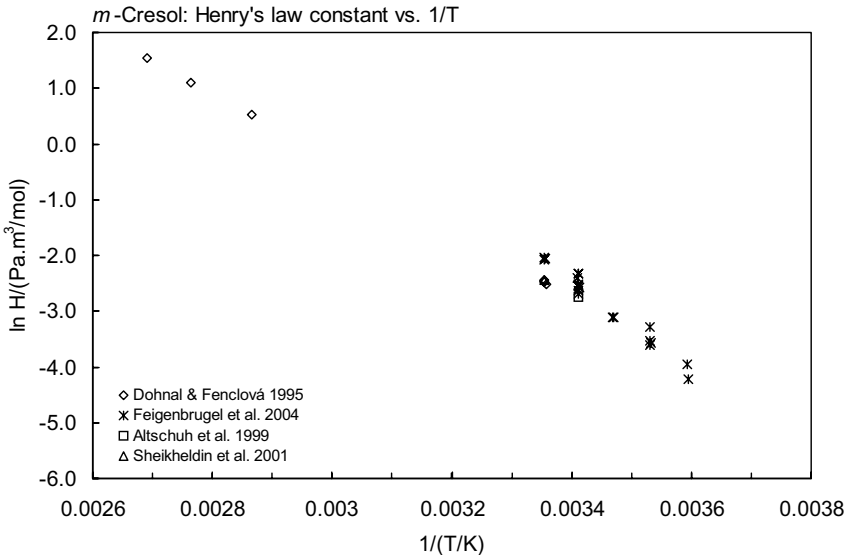

FIGURE 14.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for *m*-cresol.

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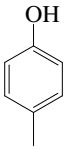
14.1.1.4 *p*-Cresol



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: C_7H_8O, $CH_3C_6H_4OH$
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, pK_a:
10.26 (Pearce & Simkins 1968, Dean 1985, Riddick et al. 1986; Howard 1989)
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, ΔH_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, ΔH_{subl} (kJ/mol):
73.93 (at 25°C, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.72 (Tsonopoulos & Prausnitz 1971; Dean 1992)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.22 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{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. γ^∞ 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)

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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) = 12.0298 – 3861.98/(t/°C + 273); temp range 0–34°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
log (P/mmHg) = 7.11767 – 1566.029/(t/°C + 167.680); temp range 110–200°C (Antoine eq. from gas-saturation-diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
133.3 (53°C, Andon et al. 1960; Haque et al. 1980)
log (P/mmHg) = [–0.2185 × 13611.7/(T/K)] + 9.190555; temp range 53–201.8°C (Antoine eq., Weast 1972–73)
11.8 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.03508 – 1511.08/(161.854 + t/°C); temp range 128–210.88°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
13.94 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 475.109/(T/K)] × 10^{1.07944 – 11.6938 × 10^{-4}·(T/K) + 9.28202 × 10^{-7}·$(T/K)^2$}; temp range: 323.20–704.65 K, (Cox eq., Chao et al. 1983)
11.8, 17.5 (calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.15637 – 1508.694/(161.594 + t/°C), temp range 128–201.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
log (P/kPa) = 6.44531 – 1713.242/(183.846 + t/°C); temp range 15.7–200.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
11.83 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.03508 – 1511.08/(161.85 + t/°C); temp range 128–202°C (Antoine eq., Dean 1985, 1992)
17.3 (Riddick et al. 1986)
15.6 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_S/kPa) = 12.098 – 3861.98/(T/K); temp range 273–307 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.16859 – 3868.314/(T/K); temp range 277–307 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.24257 – 1566.029/(–105.47 + T/K); temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.83697 – 1930.688/(–73.422 + T/K); temp range 308–393 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.2376 – 1563.08/(–105.776 + T/K); temp range 385–477 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.19164 – 1533.535/(–108.781 + T/K); temp range 463–533 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.99685 – 2310.405/(–10.362 + T/K); temp range 523–635 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
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); temp range: 397–476 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
log (P/mmHg) = 122.8998 –7.6175 × 10^3/(T/K) –41.637·log (T/K) + 1.5709 × 10^{-2}·(T/K) –8.9199 × 10^{-13}·$(T/K)^2$; temp range 308–705 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):
0.0802; 0.0699; 1.0820 (exptl., calculated-group contribution; calculated-bond contribution Hine & Mookerjee 1975)

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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. γ^{∞} 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_{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_{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. γ 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_{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_{OA}:

Bioconcentration Factor, log BCF:
1.26 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{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_{OW}, Kollig 1993)
2.70 (soil, calculated-MCI $^{1}\chi$, 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, $t_{½}$:
Volatilization: $t_{½}$ ~167 d, estimated from a lake as calculated from equations of Mackay & Wolkoff 1973 (Smith et al. 1978).
Photolysis:
$k = 6.8 \times 10^{-7}$ s^{-1} under overcast weather of April at 25°C; $t_{½}$ ~ 4800 h in river, $t_{½}$ > 10000 h in both eutrophic lake and pond and $t_{½}$ = 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 $t_{½}$ = 5800 h in aquatics (Haque et al. 1980).
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:

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photooxidation $t_{½}$ = 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)

$k_{NO3} = (13 \pm 2) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 ± 1 K (Japar & Niki 1975; Graham & Johnston 1978; quoted, Carter et al. 1981)

k(aq.) = 20 M^{-1} s^{-1}, averaged over 24-h day (Smith et al. 1978)

$k_{OH} = 38 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 ± 1 K (Atkinson et al. 1979; quoted, Carter et al. 1981)

photooxidation $t_{½}$ = 10 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson et al. 1979; quoted, Howard 1989)

$k_{NO3} = (15 \pm 2.4) \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} at 300 ± 1 K in air (relative rate technique with reference to 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

$k_{O3} = (4.71 \pm 0.66) \times 10^{-19}$ cm^3·molecule^{-1} s^{-1} at 296 ± 2 K; calculated tropospheric lifetimes of 25 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

$k = (3.0 \pm 0.6) \times 10^4$ M^{-1} s^{-1} for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{OH} = 4.50 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{NO3} = 1 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{OH} = (16.6 \pm 1.8) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 ± 1 K (relative technique with reference to *m*-cresol, Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{NO3} = (1.27 \pm 0.36) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K in air (Atkinson et al. 1984)

photooxidation $t_{½}$ = 1.5–15 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

k_{OH}(exptl) = 44.8×10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{OH}(obs.) = 41×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1985)

k_{OH}(calc) = 56.2×10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{OH}(exptl) = 42×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1985; quoted, Sabljic & Güesten 1990; Müller & Klein 1991

k_{OH}(calc) = 44×10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{OH}(exptl) = 44×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990)

$k = 1.1 \times 10^7$ M^{-1} s^{-1} at pH 8.3, 2.4×10^7 M^{-1} s^{-1} at pH 8.8, 1.6×10^8 M^{-1} s^{-1} at pH 10, 3.5×10^8 M^{-1} s^{-1} at pH 11.5 for the reaction with singlet oxygen in water at (19 ± 2)°C (Scully & Hoigné 1987)

$k_{NO3} = 21.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{OH} = 4.7 \times 10^{-1}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

$k = (9.6 \pm 2.8) \times 10^6$ M^{-1} s^{-1} for the reaction with singlet oxygen in aqueous phosphate buffer at (27 ± 1)°C (Tratnyek & Hoigné 1991)

$k_{NO3} = (10.7 \pm 1) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K, $k_{OH} = 47 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1992)

k_{OH}(calc) = 30.83×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

$k_{OH} = 5.2 \times 10^{-11}$ cm^3 mol^{-1} s^{-1}, and k_{OH}(aq.) = 1.2×10^{-10} M^{-1} s^{-1}, the calculated atmospheric lifetime τ = 0.23 d under clear sky; τ = 0.18 d under cloudy conditions at 298 K, reduced to 0.11 d due to the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis: no hydrolyzable functional groups (Smith et al. 1978).

Biodegradation: $t_{½}$ = 1–2 d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

Completely degraded by a soil microflora in 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);

$t_{½}$ = 12 h in eutrophic lake for a point source continuously discharging 1.0 µg/mL predicted by one compartment model for all processes including dilution (Smith et al. 1978); laboratory determined $k = 5.2 \times 10^{-7}$ mL cell^{-1} h^{-1} at 25°C (Smith et al. 1978)

k(calc) = 1.7 d^{-1} in river water, k = 0.8–4.7 d^{-1} in estuary water and k = 2.8–4.8 d^{-1} in marine water after a lag period (Vashon & Schwab 1982; quoted, Battersby 1990);

$t_{½}$(aq. aerobic) = 1–16 h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; selected, Howard et al. 1991)

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$t_{½}$(aq. anaerobic) = 240–672 h, based on anaerobic screening test data (Boyd et al. 1983; Horowitz et al. 1982; selected, Howard et al. 1991);

$k = 1.72 \times 10^{-17}$ mol cell^{-1} h^{-1} in pure culture system (Banerjee et al. 1984).

Biotransformation: estimated $t_{½}$ = 12 h in river, eutrophic lake and pond and $t_{½}$ > 10000 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 $t_{½}$ = 10 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);

photooxidation $t_{½}$ = 1.5–15 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 τ = 0.23 d under clear sky and τ = 0.18 d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to τ = 0.11 d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: $t_{½}$ = 0.55 h in river, $t_{½}$ = 12 h in pond and eutrophic lake, and $t_{½}$ = 2400 h in oligotrophic lake for a point source continuously discharging 1.0 µg/mL predicted by one compartment model for all processes including dilution (Smith et al. 1978; quoted, Howard 1989);

rate constant $k = (3.0 \pm 0.6) \times 10^4$ $M^{-1} \cdot s^{-1}$ for the reaction with ozone at pH 1.5/2.0 in water (Hoigné & Bader 1983b);

$t_{½}$ = 1–16 h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{½}$ = 500 h for the reaction with singlet oxygen in water at pH 8 and (19 ± 2)°C (Scully & Hoigné 1987).

Ground water: estimated half-life for cresols, $t_{½}$ = 0.01 yr at Noordwijk (Zoeteman et al. 1981); $t_{½}$ = 2–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:

$t_{½}$ = 1–16 h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{½}$ = 0.5 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 1.0 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

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TABLE 14.1.1.4.1
Reported aqueous solubilities of *p*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
40.2	22400	0	10000	25	21500
52.6	24900	20	17000	40.2	22840
63.5	28000	40	23000	75.9	43534
73.5	31900	60	30000	88.7	50064
84.0	37200	80	37000	98.5	54615
88.8	40600	100	48000	100	56146
94.0	44700	110	56000		
124.5	74200	120	72000		
139.4	151000	130	101000		
141.2	200700	140	177000		
143.5	301300	142	226000		
143.4	400800	143	264000		
141.5	506300	143.5	340000		
134.8	606100	148	380000		
111.6	719100				
77.9	704000				
37.4	836100				
27.5	844800				
17.2	852800				
8.7	868600				
9.2	879000				
10.8	900900				
17.1	946800				
20.3	960100				
24.0	922700				
27.5	983200				
29.9	990600				
33.8	1000000				
critical solution temp 143.5°C					
triple point 8.7°C					

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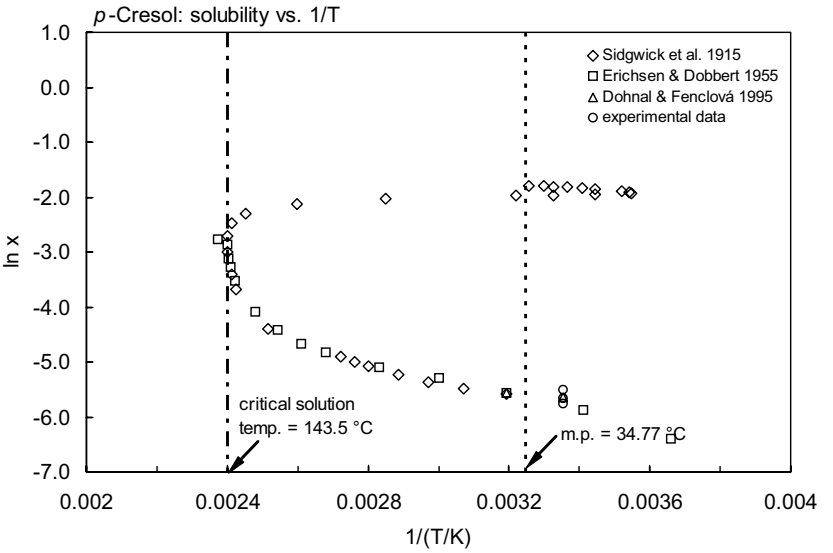

FIGURE 14.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *p*-cresol.

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)		

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
							solid		liquid
53.0	133.3	145.7	17599	128.65	7605	0	1.493	124.151	7518
76.5	666.6	163.6	32664	131.26	10114	4.75	1.640	138.025	13204
88.6	1333	171.6	42263	143.86	16500	8.60	2.653	145.593	17517
102.3	2666	179.2	53329	171.27	42066	10.8	4.066	155.395	24845
117.7	5333	187.2	67194	187.17	67661	13.9	4.880	162.723	31824
127.0	7999	193.7	80660	201.88	101325	16.8	7.199	168.937	38934
140.0	13332	200.8	98392			20.0	9.013	173.819	45366
157.7	26664	153.0	22931			22.0	12.08	178.598	52497
179.4	53329	183.8	61062	bp/°C	201.88	23.35	13.00	183.663	60995
201.8	101325	190.8	74261			28.85	21.86	186.521	66259
		197.1	88526			29.75	25.60	190.578	74355
mp/°C	35.5	200.8	98392			32.55	31.60	192.90	79336
						34.15	38.53	193.029	79631
		eq. 1	P/mmHg					197.102	89029
		A	8.308					198.609	92732
		B	2520			bp/°C	201.94	199.666	95395
								200.226	96828
						for temp range:		200.535	97964
						0–34°C		201.122	99164
						eq. 2	P/mmHg	201.719	100728
						A	12.0298	202.269	102205

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TABLE 14.1.1.4.2 *(Continued)*

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						B	3861.98	202.985	104133
						C	273		
						ΔH_V/(kJ mol^{-1})		for temp range:	
						at bp	49.534	110–200°C	
						at 25°C	73.931	eq. 2	P/mmHg
								A	7.11767
								B	1566.029
								C	167.680

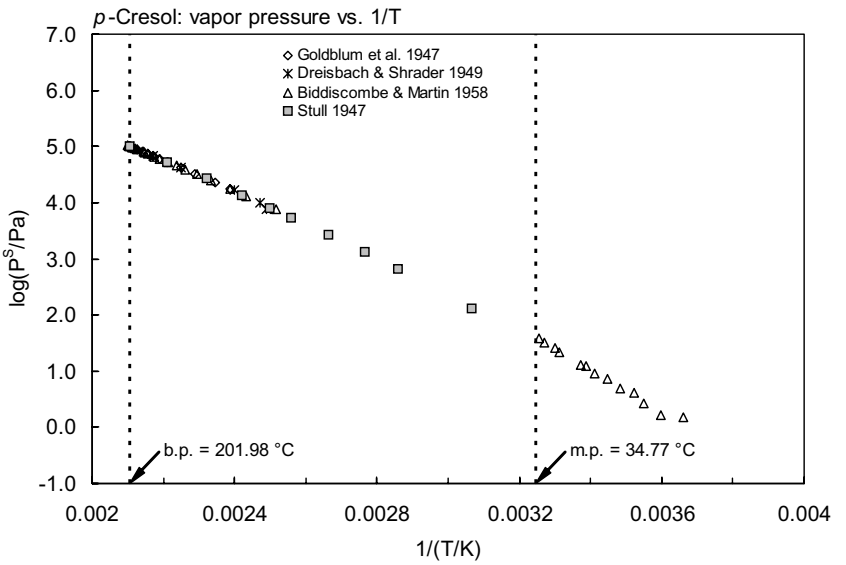

FIGURE 14.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for *p*-cresol.

TABLE 14.1.1.4.3
Reported Henry's law constants of *m*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/atm) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m^3/mol)	T/K	H/(Pa m^3/mol)
25.0	0.0783*	278.25	0.00914
40.2	0.297*	278.25	0.01148
75.9	1.735	278.35	0.00846

(Continued)

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TABLE 14.1.1.4.3 *(Continued)*

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
88.7	3.144	283.15	0.0262
98.5	4.774	283.15	0.0215
25.0	0.0801#	283.25	0.0207
25.0	0.0792$	288.10	0.0323
		288.15	0.0414
#calculated from eq. 1		288.20	0.0307
$calculated from eq. 3		293.10	0.0557
*data from literature		293.15	0.0724
		293.15	0.0627
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_K/(kJ mol^{-1}) = 48.8 ± 0.6		293	0.0582
OR		298	0.0989
eq. 3	k_H/kPa		
A	22.071		
B	6138		
ΔH_K/(kJ mol^{-1}) = 51.0 ± 0.6			

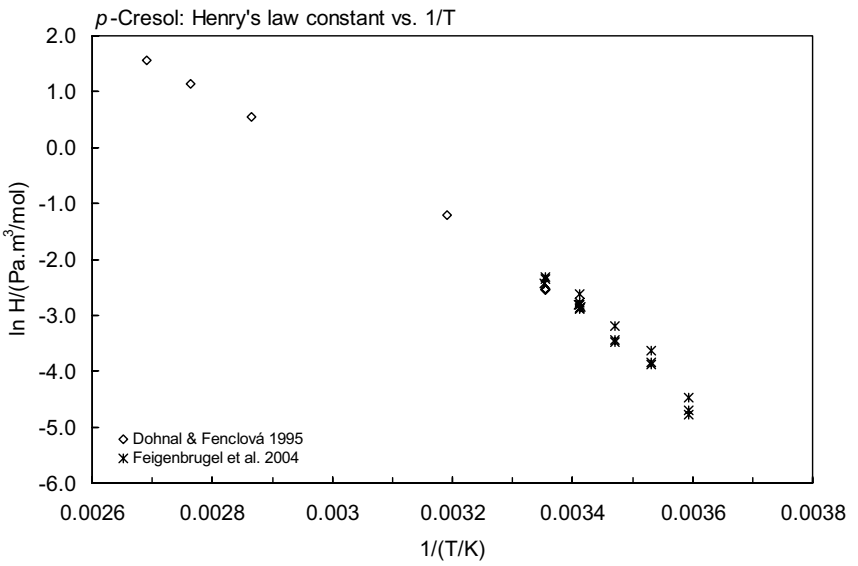

FIGURE 14.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for *p*-cresol.

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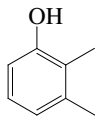
14.1.1.5 2,3-Dimethylphenol



Common Name: 2,3-Dimethylphenol
Synonym: 2,3-xylenol, 1-hydroxy-2,3-dimethylbenzene
Chemical Name: 2,3-dimetylphenol
CAS Registry No: 526-75-0
Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
72.5 (Lide 2003)
Boiling Point (°C):
216.9 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
10.54 (Dohnal & Fenclová 1995)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.08, 47.32 (25°C, normal boiling point, Andon et al. 1960)
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: 0.342 (mp at 72.5°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):
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)
3.64* (24.71°C, ebulliometry/gas saturation, measured range 10–45°C, Andon et al. 1960)
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, Boublik 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, Boublik et al. 1984)
log (P_S/kPa) = 12.29616 – 4394.694/(T/K); temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.17998 – 1619.086/(–102.197 + T/K); temp range 433–492 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = $82.92733 - 6.0367 \times 10^3/(T/K) - 26.948 \cdot \log (T/K) + 9.739 \times 10^{-3} \cdot (T/K) + 2.5196 \times 10^{-12} \cdot (T/K)^2$; temp range 346–723 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):
0.0631, 0.0952 (20, 25°C, calculated-limiting activity coefficient γ^∞ data, Dohnal & Fenclová 1995)

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2.96, 5.656, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
ln K_{AW} = 11.858 – 6567/(T/K); temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, log K_{OW}:
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, $t_{½}$, or Lifetimes, τ:

Half-Lives in the Environment:

TABLE 14.1.1.5.1
Reported aqueous solubilities of 2,3-dimethylphenol at various temperatures

Erichsen & Dobbert 1955	
shake flask-optical method	
t/°C	S/g·m^{-3}
150	40000
160	48000
170	58000
180	70000
190	94000
200	140000
202	156000
204	175000
206	200000
208	252000
208.8	365000

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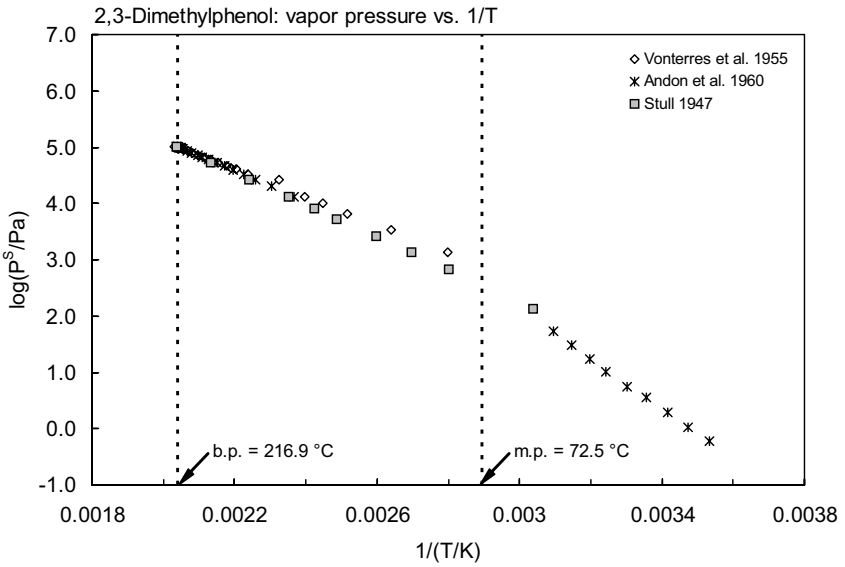

FIGURE 14.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylphenol.

TABLE 14.1.1.5.2
Reported vapor pressures of 2,3-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/mmHg) = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log (P/Pa) = A - B/(C + T/K)$	(3)		
$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		**Vonterres et al. 1955**		**Andon et al. 1960**			
summary of literature data		**ebulliometry**		**gas saturation**		**ebulliometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
56.0	133	84.0	1333	9.91	0.609	149.346	13304
83.8	666.6	105.6	3333	14.70	1.072	160.94	20045
97.6	1333	124.0	6666	19.70	1.933	169.634	26704
112.0	2666	135.2	9999	24.71	3.640	176.314	32963
129.2	5333	144.0	13332	29.58	5.650	182.500	39779
139.5	7999	157.0	26664	35.19	10.13	187.374	45920
152.2	13332	174.0	33330	39.54	17.33	192.094	53573
173.0	26664	180.2	39997	44.81	29.86	196.778	59919
196.0	53329	183.6	43330	49.88	52.93	200.752	66779
218.0	101325	186.1	46663			204.000	72842
		191.0	53329	mp/°C	72.57	207.54	79951
mp/°C	75.0	196.0	59995	bp/°C	216.87	210.672	86542
		200.0	66661			213.454	93026
		203.9	73327	for temp range:		214.137	94644
		207.0	79993	9–50°C		214.788	96151
		210.1	86659	eq. 2	P/mmHg	215.091	96929
		213.5	93325	A	13.1606	215.646	98283
		219.0	101325	B	4389.06	216.144	99513
				C	273	216.987	101613
						217.323	102400

(Continued)

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TABLE 14.1.1.5.2 *(Continued)*

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				ΔH_V/(kJ mol^{-1})		217.928	104010
				at 25°C	84.015		
				at bp	47.32	for temp range:	
						149–218°C	
						eq. 2	P/mmHg
						A	7.04268
						B	1609.184
						C	169.774

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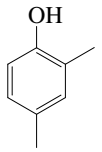
14.1.1.6 2,4-Dimethylphenol



Common Name: 2,4-Dimethylphenol
Synonym: 2,4-xylenol, *as-m*-xylenol, 1-hydroxy-2,4-dimethylbenzene
Chemical Name: 2,4-dimethylphenol
CAS Registry No: 105-67-9
Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
24.5 (Lide 2003)
Boiling Point (°C):
210.98 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0202 (Andon et al. 1960)
0.9650 (Weast 1982–83)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
10.60 (Herington & 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, ΔH_V (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, 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: 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):
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)
4200 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
7929 (calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
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)

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1333* (89.50 °C, ebulliometry, measured range 89.50–211.0 °C, Vonterres et al. 1955)
12.81* (24.87°C, ebulliometric and gas-saturation methods, measured range 9–45°C Andon et al. 1960)
13.02 (interpolated-Antoine eq. derived from exptl. results, Andon et al. 1960)
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 ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = [–0.2185 × 13130.2/(T/K)] + 8.867260; temp range 51.8–211.5°C (Antoine eq., Weast 1972–73)
10.28 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.05539 – 1587.459/(169.339 + t/°C); temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
13.17 (calculated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 483.876/(T/K)] × 10^{0.999891 – 8.94506 × 10^{-4}·(T/K) + 6.96026 × 10^{-7}·$(T/K)^2$}; temp range: 298.02–707.95 K, (Cox eq., Chao et al. 1983)
10.29, 20.22 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.18152 – 1588.34/(169.437 + t/°C), temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
log (P/kPa) = 7.02271 – 2183.475/(225.488 + t/°C); temp range 89.5–211°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
10.28 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.05539 – 1587.46/(169.34 + t/°C); temp range 144–212°C (Antoine eq., Dean 1985, 1992)
12.87 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 9.65613 – 3442.574/(T/K); temp range 282–318 K (Antoine eq.-I, 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)
12.96 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
log (P/Pa) = 86.11491 – 6138.775/(T/K) – 27.12977·log (T/K) + 0.91169 × 10^{-2}·(T/K); temp range 418–485 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
log (P/mmHg) = 53.3866 – 5.1516 × 10^3/(T/K) – 15.095·log (T/K) – 1.3196 × 10^{-9}·(T/K) + 2.8455 × 10^{-6}·$(T/K)^2$; temp range 346–708 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):

1.722 (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 m^3/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 liquid equilibrium measurements, Dohnal & Fenclová 1995)
ln K_{AW} = 10.077 – 5811/(T/K); temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
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, Staudinger & Roberts 2001)
log K_{AW} = –5.192 + 1563/(T/K); poor correlation coefficient (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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)

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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. γ from UNIFAC not considering mutual solubility of octanol and water, Arbuckle 1983)
2.95 (calculated-activity coeff. γ 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. γ 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 χ, 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, $t_{½}$:

Volatilization:

Photolysis:

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

$k < 4 \times 10^6$ M^{-1} h^{-1} for singlet oxygen, 1.1×10^8 $M^{-1} \cdot h^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{½}$ = 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 $t_{½}$ = 8.0 h in air, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; selected, Howard 1989)

$k_{OH} = 71.5 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson 1989)

photooxidation $t_{½}$ = 1.19–11.9 h, based on estimated rate constant for the reaction with OH radical in air (Howard et al. 1991)

k_{OH}(calc) = 51.06×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)

k_{OH}(calc) = 5.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = 1.06×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

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 $t_{½}$ = 0.7 d in adapted activated sludge under aerobic conditions (Mills et al. 1982);

$t_{½}$(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); $t_{½}$(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).

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Biotransformation: rate constant for bacterial transformation of 1×10^7 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: $t_{½}$ = 8.0 h, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); photooxidation $t_{½}$ = 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 $t_{½}$ = 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: $t_{½}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

TABLE 14.1.1.6.1
Reported aqueous solubilities and Henry's law constants of 2,4-dimethylphenol at various temperatures

Aqueous solubility		Henry's law constant			
Erichsen & Dobbert 1955		Ashworth et al. 1988		Dohnal & Fenclová 1995	
shake flask-optical method		EPICS-GC		vapor-liquid equilibrium	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
160	17000	10	840	75.9	4.338
170	33000	15	683	88.7	7.491
180	54000	20	1023	98.5	11.46
190	77000	25	500		
200	114000	30	380		
210	188000				
212	234000	log H = A – B/(T/K)			
213	279000		H/(atm m^3/mol)		
213.5	335000	A	–16.34		
25	6200	B	–3307		
	extrapolated				

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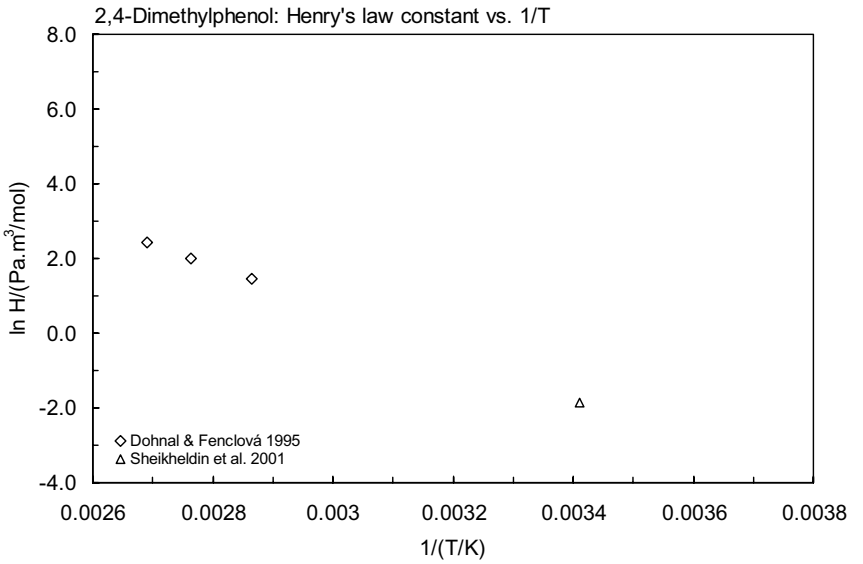

FIGURE 14.1.1.6.1 Logarithm of Henry's law constant versus reciprocal temperature for 2,4-dimethylphenol.

TABLE 14.1.1.6.2
Reported vapor pressures of 2,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log (P/mmHg) = A - B/(C + t/°C)$ (2)
$\log (P/Pa) = A - B/(C + T/K)$ (3)
$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.50	1333	9.73	3.040	144.382	13195
78.0	666.6	109.9	3333	14.94	5.066	156.053	20024
91.3	1333	127.0	6666	20.13	8.279	164.129	26289
105	2666	137.4	9999	24.87	12.81	171.241	33051
131.5	5333	144.5	13332	29.91	20.13	176.700	39155
131	7999	156.0	19998	35.16	30.797	182.116	46078
143	13332	165.1	26664	39.41	43.73	186.169	52557
161.5	26664	171.2	33330	44.86	67.06	191.348	60131
184.5	53329	177.3	39997			194.795	66188
211.5	101325	180.0	46663	mp/°C	24.54	198.444	73115
		186.7	53329	bp/°C	210.931	201.747	79877
mp/°C	25.5	190.8	59995			204.809	86584
		194.4	66661	for temp range:		207.513	92867
		198.0	73327	9–45°C		208.299	94764
		201.0	79993	eq. 2	P/mmHg	208.898	97557
		204.0	86659	A	10.5277	209.314	97251
		206.6	93325	B	3499.99	209.847	98580
		211.0	101325	C	273	210.45	100102
						210.951	101381

(Continued)

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TABLE 14.1.1.6.2 *(Continued)*

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				ΔH_V/(kJ mol^{-1})		211.453	102666
				at 25°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

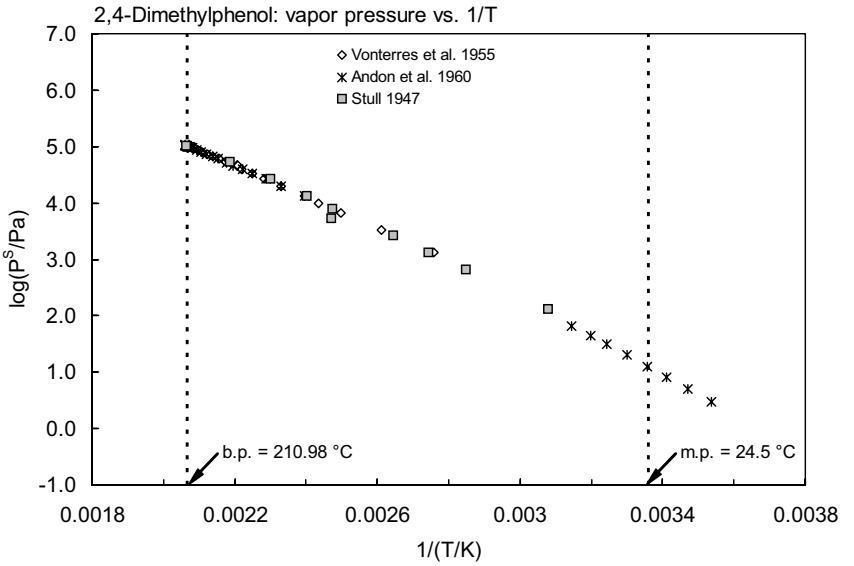

FIGURE 14.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dimethylphenol.

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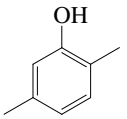
14.1.1.7 2,5-Dimethylphenol



Common Name: 2,5-Dimethylphenol
Synonym: 2,5-xylenol, 1-hydroxy-2,5-dimethylbenzene
Chemical Name: 2,5-dimethyl phenol
CAS Registry No: 95-87-4
Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
74.8 (Lide 2003)
Boiling Point (°C):
211.1 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
10.41 (Dohnal & Fenclová 1995)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
84.98, 46.94 (25°C, normal bp, Andon et al. 1960)
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: 0.325 (mp at 74.8°C)

Water Solubility (g/m^3 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* (89.40 °C, ebulliometry, measured range 89.40–211.2°C, Vonterres 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, Boublik 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 Vonterres et al. 1955, Boublik et al. 1984)
log (P_S/kPa) = 12.51064 – 3950.681/(T/K), temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/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 × 10^3/(T/K) –13.186·log (T/K) – 1.0208 × 10^{-9}·(T/K) + 2.7045 × 10^{-12}·(T/K)^2; temp range 348–707 K (vapor pressure eq., Yaws 1994)

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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):

0.0873, 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, $t_{½}$:

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

log P = A – B/(T/K) (1)
log (P/mmHg) = A – B/(C + t/°C) (2)
log (P/Pa) = A – B/(C + T/K) (3)
log (P/mmHg) = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.40	1333	9.42	0.60	143.024	12990
78.0	666.6	109.8	3333	15.01	1.215	154.805	19234
91.3	1333	126.8	6666	19.9	2.186	164.433	26584
105	2666	137.2	9999	24.82	3.946	171.549	33375
121.5	5333	144.5	13333	29.83	6.849	176.902	39361
131	7999	156.0	19998	35.33	12.59	182.455	46460
143	13332	164.8	26666	39.41	19.47	187.328	53509
161.5	26664	171.5	33330	44.79	34.53	191.46	60142
184.2	53329	177.4	39997	49.75	52.80	194.984	66312
211.5	101325	180.2	43330			198.93	73602
		182.5	46663			210.834	79735
mp/°C	74.5	186.6	53329	mp/°C	74.85	204.603	85737
		189.5	59995	bp/°C	211.132	207.748	92988
		194.2	66661			208.661	95182
		198.0	73327	for temp range:		209.138	96349
		201.0	79993	9–50°C		209.556	97373

(Continued)

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TABLE 14.1.1.7.1 *(Continued)*

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		204.6	86659	eq. 2	P/mmHg	210.117	98764
		206.8	93325	A	13.3705	210.771	100257
		211.2	101325	B	4438.56	211.232	101580
				C	273	211.736	102870
				ΔH_V/(kJ mol^{-1})		for temp range:	
				at 25°C	84.98	143–212°C	
				at bp	46.94	eq. 2	P/mmHg
						A	7.03684
						B	1581.906
						C	169.497

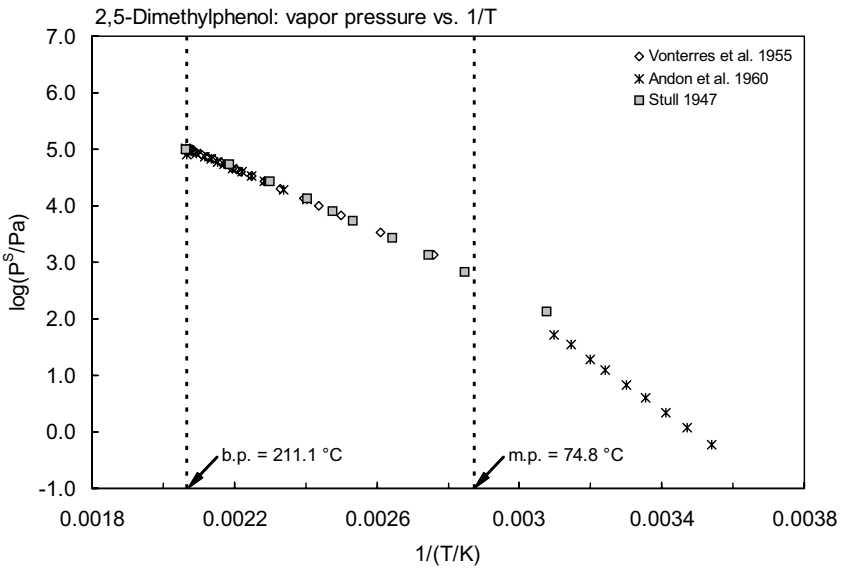

FIGURE 14.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for 2,5-dimethylphenol.

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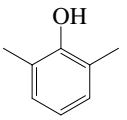
14.1.1.8 2,6-Dimethylphenol



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: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
45.8 (Lide 2003)
Boiling Point (°C):
201.07 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1320 (25°C, Andon et al. 1960)
Molar Volume (cm^3/mol):
107.9 (25°C, calculated-density)
147.8 calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
10.60 (McLeese et al. 1979; Dean 1985; Varhaníčková et al. 1995)
10.63 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
60.41, 46.97 (25°C, bp, Dreisbach 1955)
44.52 (at normal boiling point, Andon et al. 1960)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
75.6 (at 25°C, Andon et al. 1960; Dean 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.9; 16.3 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 0.625 (mp at 45.8°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):
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, Wasik 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, Vonterres 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)

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34.41 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.0707 – 1628.323/(187.603 + t/°C), temp range 144.8–203.5°C (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/mmHg) = [1– 474.112/(T/K)] × 10^{0.99333 – 9.96552 × 10^{-4}·(T/K) + 8.34247 × 10^{-7}·$(T/K)^2$}; temp range 321.81–701.65 K (Cox eq., Chao et al. 1983)
34.41, 10.37 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.19572 – 1628.413/(187.613 + t/°C), temp range 144.8–203.5°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
log (P/kPa) = 6.57979 – 1831.266/(188.83 + t/°C), temp range 97.5–212°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
34.4 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.00707 – 1628.32/(187.60 + t/°C); temp range 145–204°C (Antoine eq., Dean 1985, 1992)
19.09 (selected, Riddick et al. 1986)
24.0 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.6308 – 3950.681/(T/K); temp range 277–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.19544 – 1629.621/(–85.358 + T/K); temp range 417–476 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
43.8 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
log (P/Pa) = 39.83138 – 4062.725/(T/K) – 10.16994·log (T/K) + 0.20170 × 10^{-2}·(T/K); temp range: 418–477 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
log (P/mmHg) = 87.1964 – 5.8721 × 10^3/(T/K) – 28.853·log (T/K) + 1.113 × 10^{-2}·(T/K) + 2.2316 × 10^{-12}·$(T/K)^2$; temp range 319–701 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):
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_{AW} = 11.176 – 5906/(T/K), temp range 20–100°C (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, $t_{½}$:
Volatilization:
Photolysis:

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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:
$k_{OH} = 65.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1989)
k_{OH}(calc) $= 54.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} estimated from Atmospheric Oxidation Program, k_{OH}(exptl) $= 65.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}; and k_{OH}(calc) $= 30.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} estimated from Fate of Atmospheric Pollutants Program (Meylan & Howard 1993)
k_{OH}(calc) $= 49.48 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital estimation method, Klamt 1993)
Hydrolysis:
Biodegradation: $t_{½}$ = 7–10 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:

Half-Lives in the Environment:

TABLE 14.1.1.8.1
Reported aqueous solubilities and vapor pressures of 2,6-dimethylphenol at various temperatures

log P = A – B/(T/K) (1)
log (P/mmHg) = A – B/(C + t/°C) (2)
log (P/Pa) = A – B/(C + T/K) (3)
log (P/mmHg) = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
130	13000	92.5	1333	4.75	2.60	144.798	19813
140	16000	112.5	3333	9.46	4.48	153.385	26322
150	21000	129.0	6666	14.98	8.319	160.524	33079
160	27000	139.4	9999	19.78	13.87	166.759	39853
170	36000	147.1	13332	24.67	23.33	171.831	46274
180	47000	158.4	19998	30.2	39.86	176.276	52564
190	58000	167.0	26664	34.98	64.93	180.369	59847
200	71000	173.2	33330	39.66	100.3	184.792	66529
210	90000	179.1	39997			188.694	73851
220	120000	181.5	43330	mp/°C	74.85	191.754	80043
230	176000	188.0	53329	bp/°C	201.03	194.81	86616
232	191000	190.2	59995			196.676	90843
234	209000	196.3	66661	for temp range:		198.414	94918
236	229000	200.0	73327	4–40°C		198.937	96176
238	255000	202.5	79993	eq. 2	P/mmHg	199.432	97373
240	297000	205.6	86659	A	12.5036	199.983	98721
241.2	440000	208.0	93325	B	3948.27	200.45	99881
		212.0	101325	C	273	201.059	101400
						201.616	120808
				ΔH_V/(kJ mol^{-1})		202.519	105117
				at 25°C	75.60	203.525	107738
				at bp	44.52		

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TABLE 14.1.1.8.1 *(Continued)*

Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						for temp range:	
						144–203°C	
						eq. 2	P/mmHg
						A	7.05753
						B	1618.528
						C	186.492

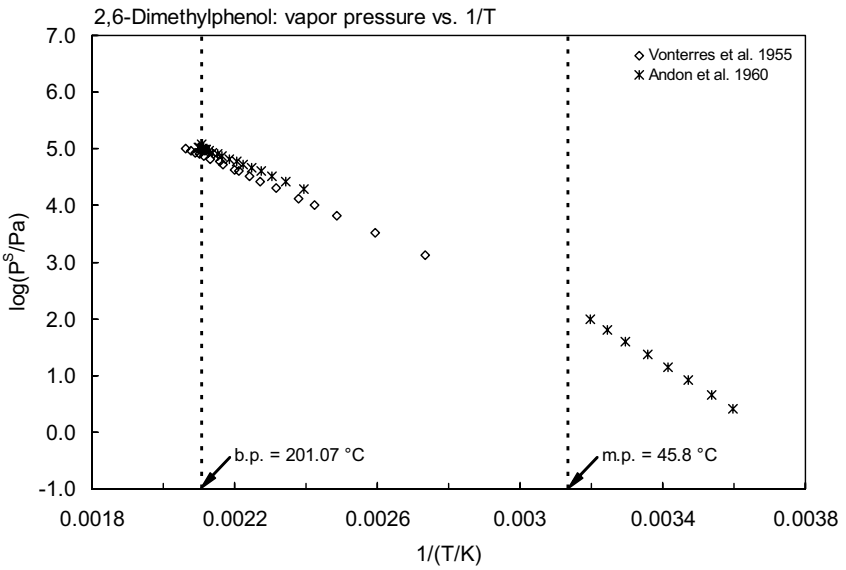

FIGURE 14.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dimethylphenol.

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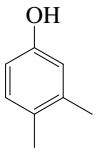
14.1.1.9 3,4-Dimethylphenol



Common Name: 3,4-Dimethylphenol
Synonym: 3,4-xylenol, *as-o*-xylenol
Chemical Name: 3,4-dimethylphenol
CAS Registry No: 95-65-8
Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
65.1 (Lide 2003)
Boiling Point (°C):
227 (Lide 2003)
Density (g/cm^3 at 20°C):
1.1380 (25°C, Andon et al. 1960)
0.9830 (Weast 1982–83)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
10.40 (McLeese et al. 1979)
10.32 (Dean 1985)
10.36 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
49.67 (at normal boiling point, Andon et al. 1960)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
85.73 (at 25°C, Andon et al. 1960; Dean 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.13; 17.0 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.404 (mp at 65.1°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):
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)

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1333* (105.7 °C, ebulliometry, measured range 105.7–226.0°C, Vonterres et al. 1955)
1.84* (24.88°C, ebulliometry/gas-saturation methods, measured range 9.89–49.36°C, Andon et al. 1960)
1.895 (interpolated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)
log (P/mmHg) = 13.1729 – 4478.23/(t/°C + 273); temp range: 9–50°C, (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = 7.07343 – 1617.202/(t/°C + 158.778); temp range 171–229°C (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)
log (P/mmHg) = [–0.2185 × 13991.0/(T/K)] + 9.02680; temp range 66.2–225.2°C (Antoine eq., Weast 1972–73)
2.541 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.07979 – 1621.451/(159.261 + t/°C); temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
3.621 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 499.926/(T/K)] × 10^{1.05062 – 10.2129 × 10^{-4}·(T/K) + 8.04338 × 10^{-7}·$(T/K)^2$}; temp range: 353.20–729.65 K, (Cox eq., Chao et al. 1983)
7.327 (supercooled liquid P_L, extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.20545 – 1622.411/(159.947 + t/°C); temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
log (P/kPa) = 7.46831 – 2538.736/(239.359 + t/°C); temp range 105.7–226°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
2.540 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.07919 – 1621.45/(159.26 + t/°C); temp range 172–229°C (Antoine eq., Dean 1985, 1992)
5.160 (Riddick et al. 1986)
1.865 (solid P_S, interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 12.31521 – 4485.592/(T/K); temp range 282–323 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.20617 – 1623.592/(–113.623 + T/K); temp range 444–502 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
3.795 (extrapolated-four parameter vapor pressure eq., Nesterova et al. 1990)
log (P/Pa) = 93.28460 – 6735.317/(T/K) – 29.48566·log (T/K) + 0.95432 × 10^{-2}·(T/K); temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1950, Nesterova et al. 1990)
log (P/mmHg) = 68.6521 – 6.15 × 10^3/(T/K) – 20.184·log (T/K) – 1.1259 × 10^{-10}·(T/K) + 4.0266 × 10^{-6}·$(T/K)^2$; temp range 338–730 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):

0.00942 (Leuenberger et al. 1985)
0.0212 (calculated-P/C, Shiu et al. 1994)
0.0278 (20°C, calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
1.416, 2.903, 4.619 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
0.0421 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
ln K_{AW} = 11.854 – 6809/(T/K), temp range 20–100°C (vapor-liquid equilibrium VLE measurements with additional lit. data, Dohnal & Fenclová 1995)
0.098 (calculated-group contribution, Lee et al. 2000)

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

2.23 (20°C, shake flask-UV, Korenman 1973)
2.23 (shake flask, Korenman et al. 1980)
2.23 (recommended, Sangster 1989, 1993)
2.23 (recommended, Hansch et al. 1995)
2.36 (HPLC-RT correlation, Makovskaya et al. 1995b)
2.26 (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}:

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = 81.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (Atkinson 1989)
k_{OH}(calc) = 55.1×10^{-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	
shake flask-optical method	
t/°C	S/g·m^{-3}
130	29000
140	36000
150	42000
160	59000
170	81000
180	124000
186	173000
188	200000
189	222000
190	278000
190.2	336000
25	5100*

*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

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log (P/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.2	133.3	105.7	1333	9.89	0.293	171.933	20341
93.8	666.6	125.8	3333	14.78	0.543	180.131	26703
107.7	1333	142.6	6666	19.98	1.031	186.548	32749

(Continued)

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TABLE 14.1.1.9.2 *(Continued)*

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
122	2666	152.9	9999	24.88	1.840	193.38	40369
138	5333	160.9	13332	29.8	3.240	197.879	46135
148	7999	172.3	19998	34.86	5.626	202.37	52526
162	13332	180.3	26664	39.67	9.386	207.376	60478
181.5	26664	187.7	33330	44.76	16.13	211.126	67049
203.6	53329	193.9	39997	49.36	25.46	213.126	72703
225.2	101325	196.3	43330			217.587	79685
		198.7	46663	mp/°C	65.11	200.898	86882
mp/°C	62.8	203.0	53339	bp/°C	221.692	223.649	93227
		212.5	66661			224.292	94764
		213.4	73327	for temp range:		224.799	95996
		216.5	79993	9–50°C		225.276	97153
		219.2	86659	eq. 2	P/mmHg	225.928	98771
		222.0	93325	A	13.1729	226.392	99920
		226.0	101325	B	4478.23	226.921	101242
				C	273	227.397	102474
						228.487	105289
				ΔH_V/(kJ mol^{-1})		228.899	106371
				at 25°C	85.73		
				at bp	49.67	for temp range:	
						171–229°C	
						eq. 2	P/mmHg
						A	7.07343
						B	1617.202
						C	158.778

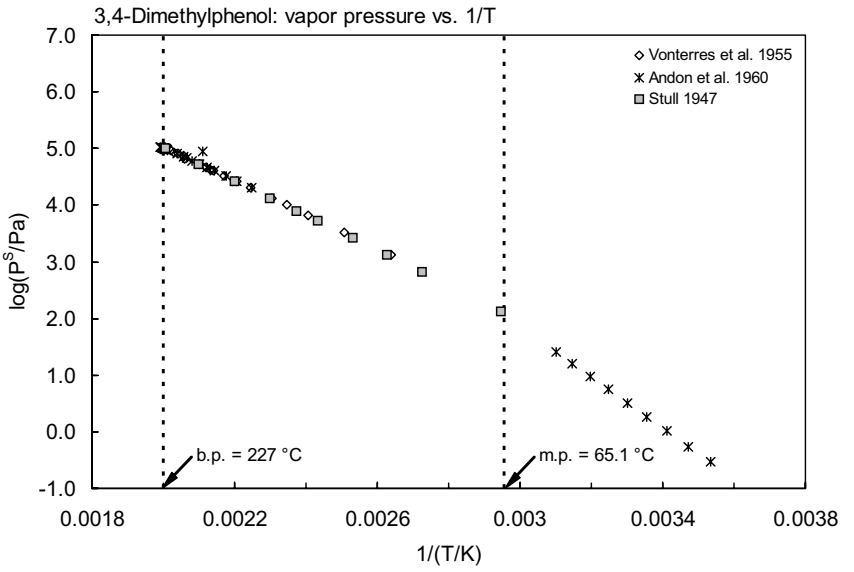

FIGURE 14.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 3,4-dimethylphenol.

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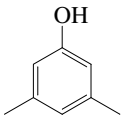
14.1.1.10 3,5-Dimethylphenol



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: $C_8H_{10}O$ $CH_3C_6H_3(CH_3)OH$
Molecular Weight: 122.164
Melting Point (°C):
63.4 (Lide 2003)
Boiling Point (°C):
221.74 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constants, pK_a:
7.8 (McLeese et al. 1979)
10.19 (Dohnal & Fenclová 1995)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
82.84, 49.31 (25°C, normal bp, Andon et al. 1960)
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: 0.420 (mp at 63.4°C)

Water Solubility (g/m^3 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, Vonterres et al. 1955)
2.63* (24.95°C, ebulliometry/gas saturation, measured range 9–45°C, Andon 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/mmHg) = 7.11745 – 1630.124/(t/°C + 163.076); temp range 154–224°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 exptl data of Andon et al. 1960, Boublik et al. 1984)
log (P/kPa) = 8.27972 – 3182.232/(287.862 + t/°C), temp range 102.8–219°C (Antoine eq. derived from reported exptl data of Vonterres et al. 1960, Boublik et al. 1984)
log (P_S/kPa) = 11.97153 – 4336.025/(T/K); temp range 282–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.25292 – 1638.564/(–109.095 + T/K); temp range 427–497 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = $-44.915 - 2.8912 \times 10^3/(T/K) + 25.704 \cdot \log (T/K) - 3.9714 \times 10^{-2} \cdot (T/K) + 1.6464 \times 10^{-5} \cdot (T/K)^2$; temp range 337–716 K (vapor pressure eq., Yaws 1994)

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Henry's Law Constant (Pa m^3/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 K_{AW} = 11.654 – 6636/(T/K); temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

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

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 K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log (P/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
62	133.3	102.8	1333	9.57	0.44	154.72	12984
89.2	666.6	122.5	3333	14.92	0.813	166.472	19760
102.4	1333	139.1	6666	20.35	1.587	175.126	26444
117.0	2666	149.0	9999	24.05	2.626	182.389	33392
133.3	5333	156.8	13332	30.42	4.866	187.937	39757
143.5	7999	168.1	19998	34.85	7.813	192.743	45815
156	13332	176.3	26664	39.94	13.32	197.298	52352
176.2	26664	182.9	33330	45.23	22.80	201.925	59794
197.8	53329	188.5	39997	49.97	35.33	205.601	66193
219.5	101325	191.0	43330			209.151	72942
		194.0	46663			212.159	79072
mp/°C	68.0	198.1	53329	mp/°C	63.27	215.799	87070
		202.0	59995	bp/°C	221.692	218.298	92904
		205.3	66661			219.146	94952
		208.3	73327	for temp range:		219.584	96027
		211.0	79993	9–50°C		220.097	97296
		214.0	86659	eq. 2	P/mmHg	220.692	98771

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TABLE 14.1.1.10.1 *(Continued)*

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		216.2	93325	A	12.8271	221.309	100334
		219.0	101325	B	4328.13	221.709	101362
				C	273	222.269	102845
						222.724	104007
				ΔH_V/(kJ mol^{-1})		223.321	105573
				at 25°C	82.84		
				at bp	49.31	for temp range:	
						154–224°C	
						eq. 2	P/mmHg
						A	7.11745
						B	1630.124
						C	163.076

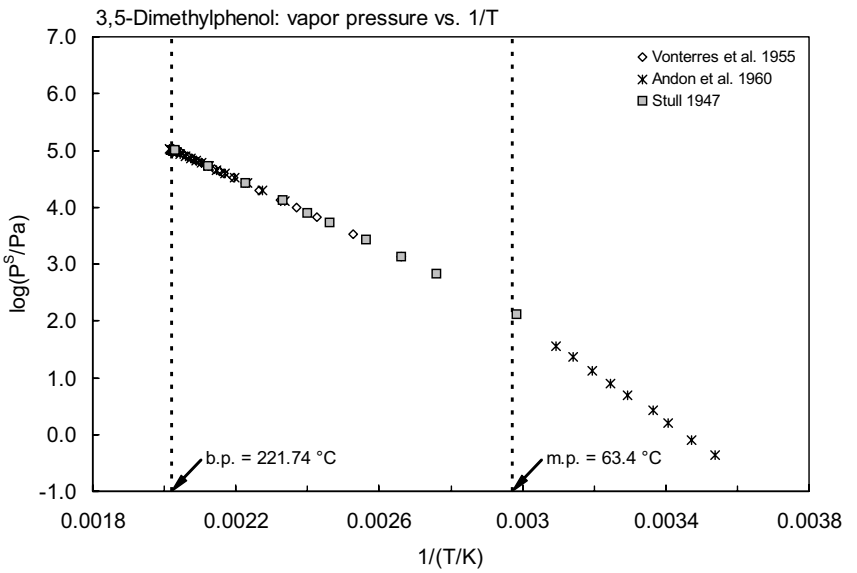

FIGURE 14.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 3,5-dimethylphenol.

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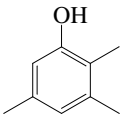
14.1.1.11 2,3,5-Trimethylphenol



Common Name: 2,3,5-Trimethylphenol
Synonym:
Chemical Name: 2,3,5-trimethylphenol
CAS Registry No: 697-82-5
Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$
Molecular Weight: 136.190
Melting Point (°C):
94.5 (Lide 2003)
Boiling Point (°C):
233 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
10.60 (Blackman et al. 1955)
Molar Volume (cm^3/mol):
170.0 (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: 0.208 (mp at 94.5°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):
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., ebulliometric method, Handley et al. 1964)
4.451 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1–508.477/(T/K)] × 10^{0.932965 – 5.75276 × 10^{-4}·(T/K) + 3.29737 × 10^{-7}·(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 exptl. 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 exptl. 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 exptl. 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 (P_L/kPa) = 6.20676 – 1687.869/(–106.761 + T/K), temp range 459–531 K (Antoine eq., Stephenson & Malanowski 1987)

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log (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-m^3/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 $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

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

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa
200	40000	186.482	26547
210	54000	193.614	33021
220	79000	200.127	40002
230	128000	205.448	46560
240	200000	210.422	53453
242	224000	214.675	59972
244	250000	218.644	66623
246	291000	222.382	73417
257.8	420000	225.707	79909
		229.041	86877
		231.852	93116
		234.759	99940
		237.50	106735
		240.13	113587
		242.511	120090
		244.811	126646
		247.062	133344
		mp/°C	93.73
		bp/°C	235.329

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TABLE 14.1.1.11.1 *(Continued)*

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa
		for temp range:	
		186–247°C	
		log (P/mmHg) = A – B/(C + t/°C)	
			P/mmHg
		A	7.08022
		B	1685.973
		C	166.150
		ΔH_V/(kJ mol^{-1})	
		at bp	49.96

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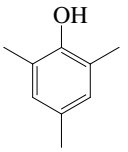
14.1.1.12 2,4,6-Trimethylphenol



Common Name: 2,4,6-Trimethylphenol
Synonym: Mesitol
Chemical Name: 2,4,6-Trimethylphenol
CAS Registry No: 527-60-6
Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$
Molecular Weight: 136.190
Melting Point (°C):
73 (Lide 2003)
Boiling Point (°C):
220 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
10.90 (Blackman et al. 1955)
10.88 (Dean 1985)
Molar Volume (cm^3/mol):
170.0 (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: 0.338 (mp at 73°C)

Water Solubility (g/m^3 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)
log (P/kPa) = 5.91352 – 1481.329/(158.589 + t/°C), temp range 94–220.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
19.6 (supercooled liquid P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.82395 – 2158.2/(–45.2 + T/K), temp range 367–494 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/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, $t_{½}$:

Half-Lives in the Environment:

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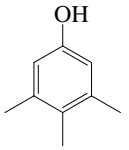
14.1.1.13 3,4,5-Trimethylphenol



Common Name: 3,4,5-Trimethylphenol
Synonym:
Chemical Name: 3,4,5-trimethylphenol
CAS Registry No: 527-54-8
Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$
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/cm^3):
Acid Dissociation Constant, pK_a:
10.25 (Dean 1985)
Molar Volume (cm^3/mol):
170.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.153 (mp at 108°C)

Water Solubility (g/m^3 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 (P_L/kPa) = 7.33216 – 2536.1/(–44.56 + T/K), temp range 396–521 K (Antoine eq., Stephenson & Malanowski 1987)

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

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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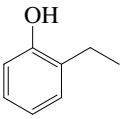
14.1.1.14 *o*-Ethylphenol



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): 204.52
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 (Verschueren 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, 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/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), 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); 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 + 170.833); temp range 150–218°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)
log (P/mmHg) = [–0.2185 × 12516.7/(T/K)] + 8.586948; temp range 46.2–207.5°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = [1– 480.731/(T/K)] × 10^{0.883881 – 6.07675 × 10^{-4}·(T/K) + 6.44264 × 10^{-7}·$(T/K)^2$}; temp range: 319.35–480.65 K, (Cox eq., Chao et al. 1983)
16.7, 29 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.13214 – 1548.802/(170.82 + t/°C), temp range 150.4–215.05°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)
log (P/kPa) = 6.97225 – 2178.815/(231.035 + t/°C), temp range 86–207.5°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
27.01 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 7.8003 – 2140.4/(227 + t/°C), temp range 86–208°C (Antoine eq., Dean 1985, 1992)
20.87 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

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log (P_L/kPa) = 6.13344 – 1550.409/(–102.103 + T/K); temp range 423–491 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)
log (P_L/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·log (T/K) + 1.09475 × 10^{-2}·(T/K); temp range: 424–491 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

Henry's Law Constant (Pa·m^3/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, $t_{½}$:

Half-Lives in the Environment:

TABLE 14.1.1.14.1
Reported vapor pressures of *o*-ethylphenol 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/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Biddiscombe et al. 1963			
summary of literature data		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
46.2	133.3	4.98	3.346	150.425	20458
73,4	666.6	10.0	5.173	158.137	26542
87	1333	15.01	8.759	164.876	32996
101.5	2666	20.01	13.73	171.143	40086
117.9	5333	24.93	20.40	176.174	46627
127.9	7999	29.53	30.80	180.808	53390
141.8	13332	34.84	45.86	184.869	59946
161.6	26664	39.99	73.99	188.565	66460
184,5	53329	45.0	102.9	192.115	73235
207.5	101325			195.266	79702
				198.382	86528
mp/°C	–45	mp/°C	–3.31	200.845	92242

(Continued)

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	bp/°C	217.985	204.350	100866

TABLE 14.1.1.14.1 *(Continued)*

Stull 1947		Biddiscombe et al. 1963			
summary of literature data		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				206.632	106865
		for temp range:		208.429	111753
		5–45°C		209.854	115762
		eq. 2	P/mmHg	212.651	123942
		A	10.3131	215.149	131641
		B	3313.50	218.047	142363
		C	273		
		ΔH_V/(kJ mol^{-1})		for temp range:	
		at 25°C	63.60	150–218°C	
		at bp	48.116	eq. 2	P/mmHg
				A	7.00742
				B	1548.923
				C	170.833

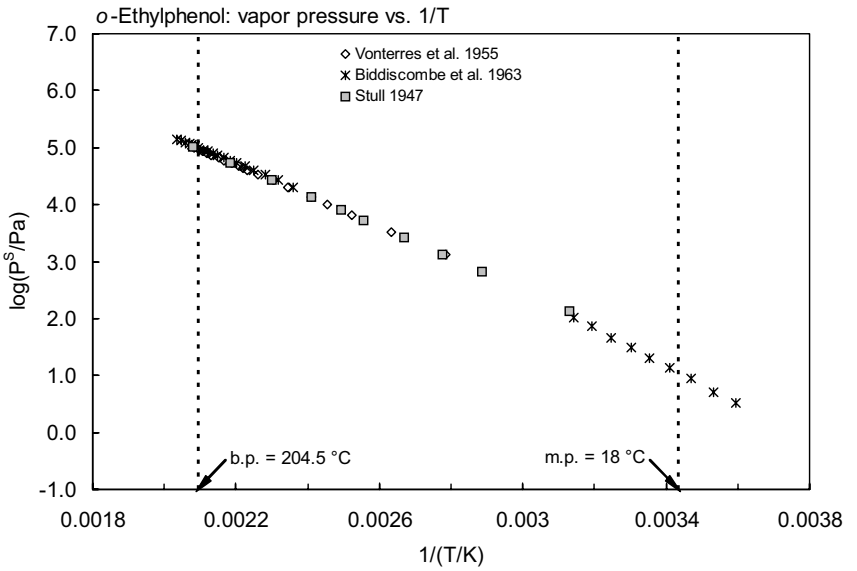

FIGURE 14.1.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for *o*-ethylphenol.

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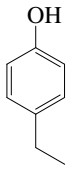
14.1.1.15 *p*-Ethylphenol



Common Name: 4-Ethylphenol
Synonym: *p*-ethylphenol
Chemical Name: 2-ethylphenol, *p*-ethylphenol
CAS Registry No: 123-07-9
Molecular Formula: $C_8H_{10}O$, $C_2H_5C_6H_4OH$
Molecular Weight: 122.164
Melting Point (°C):
45 (Lide 2003)
Boiling Point (°C):
217.9 (Lide 2003)
Density (g/cm^3 at 20°C):
1.054 (25°C, Biddiscombe et al. 1963)
1.011 (25°C, Dean 1985)
Molar Volume (cm^3/mol):
147.8 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
10.0 (Dean 1985)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
50.84 (at normal boiling point, Biddiscombe et al. 1963)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
80.33 (at 25°C, Andon et al. 1960)
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: 0.636 (mp at 45°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):
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, Vonterres 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)

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log (P/mmHg) = [–0.2185 × 13437.9/(T/K)] + 8.854990; temp range 59.3–219°C (Antoine eq., Weast 1972–73)
6.575 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.13614 – 1547.614/(156.677 + t/°C), temp range 171.8–229.1°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)
log (P/kPa) = 7.59041 – 2575.507/(242.273 + t/°C), temp range 101–218.2°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
7.530 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 8.291 – 2423/(229 + t/°C), temp range 101–218°C (Antoine eq., Dean 1985, 1992)
4.95 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.74364 – 4188.624/(T/K), temp range 278–317 K, (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.13939 – 1550.479/(–116.1 + T/K), temp range: 444–503 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
6.137 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
log (P/Pa) = 96.72774 – 6779.787/(T/K) – 30.80658·log (T/K) + 1.101581×10^{-2}·(T/K); 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/mmHg) = 16.9092 – 3.7255×10^{3}/(T/K) – 1.7886·log (T/K) – 4.2275×10^{-3}·(T/K) + 1.8002×10^{-6}·$(T/K)^2$; temp range 318–716 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.132 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.75 (literature average, Leo et al. 1971)
2.58 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
2.26 (shake flask, Korenman 1972, Korenman et al. 1980)
2.26, 2.58 (Hansch & Leo 1979)
2.60 (shake flask-UV, Rogers & Wong 1980)
2.37 (HPLC-RT correlation, Butte et al. 1981)
2.12, 2.19 (RP-HPLC-k′ correlation, Miyake & Terada 1982)
2.59 ± 0.07; 2.58 (HPLC-RV correlation-ALPM, selected best lit. value, Garst & Wilson 1984)
2.50 (recommended, Sangster 1989, 1993)
2.50 (COMPUTOX databank, Kaiser 1993)
2.40; 2.58 (pH 7.4, pH 5.6, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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TABLE 14.1.1.15.1
Reported aqueous solubilities of *p*-ethylphenol at various temperatures

Erichsen & Dobbert 1955	
synthetic method, SF-optical	
t/°C	S/g·m^{-3}
150	24000
160	30000
170	45000
180	93000
182	112000
184	141000
186	197000
187.1	395000

TABLE 14.1.1.15.2
Reported vapor pressures of *p*-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log (P/mmHg) = A - B/(C + t/°C)$ (2)
$\log (P/Pa) = A - B/(C + T/K)$ (3)
$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		Vonterres et al. 1955		Biddiscombe et al. 1963			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
59.3	133.3	101.0	1333	5.0	0.480	171.757	26571
86.5	666.6	109.8	3333	10.0	0.907	178.525	33069
100.2	1333	137.5	6666	15.0	1.613	184.585	39942
115.0	2666	148.0	9999	19.99	2.813	189.724	46636
131.3	5333	155.5	13332	25.03	4.960	194.356	53416
141.7	7999	167.0	19998	30.02	8.426	198.419	59999
154.2	13332	177.2	26664	35.0	14.27	202.227	66736
175.0	26664	182.0	33330	39.99	23.33	205.607	73211
197.4	53329	187.7	39997	43.97	34.13	208.892	79979
219.0	101325	190.5	43330			211.911	86626
		192.6	46663			214.673	93090
mp/°C	46.5	197.0	53329	mp/°C	45.06	217.535	100174
		201.7	59995	bp/°C	217.985	220.026	106683
		204.0	66661			222.543	113599
		207.4	73327	for temp range:		224.769	119995
		210.9	79993	5–44°C		226.933	126484
		213.1	86659	eq. 2	P/mmHg	229.147	133418
		216.1	93325	A	12.6090		
		218.2	101325	B	4183.81	for temp range:	
				C	273	171–229°C	
						eq. 2	P/mmHg
				ΔH_V/(kJ mol^{-1})		A	7.01297
				at 25°C	80.33	B	1548.754
				at bp	50.84	C	156.820

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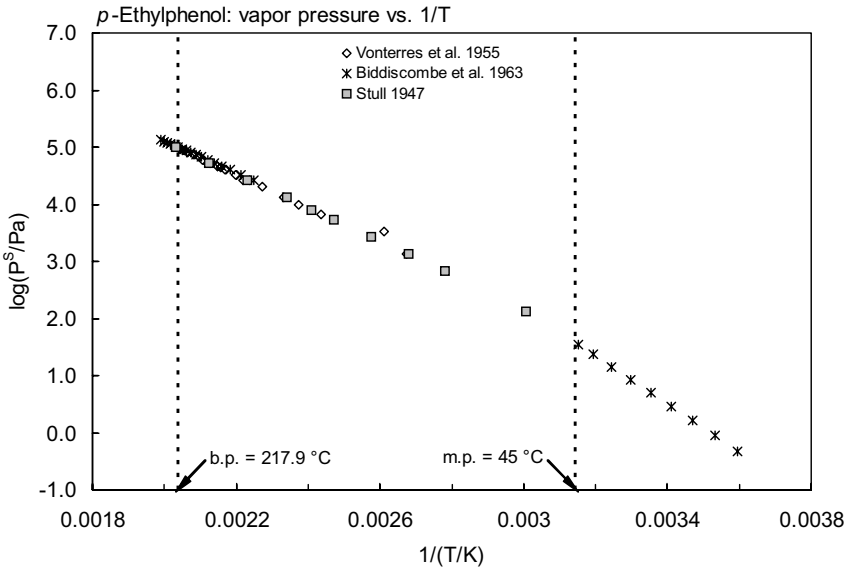

FIGURE 14.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-ethylphenol.

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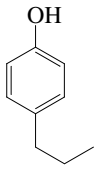
14.1.1.16 4-Propylphenol



Common Name: 4-Propylphenol
Synonym:
Chemical Name: 4-propylphenol
CAS Registry No: 645-56-7
Molecular Formula: $C_9H_{12}O$, $C_3H_7C_6H_4OH$
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/cm^3 at 20°C):
1.009 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
170.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1278 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P_L/kPa) = 7.32632 – 2550.1/(–28.65 + T/K), temp range 383–508 K, (Antoine eq., Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, log K_{OW}:
2.1 (HPLC-RT correlation, McLeese et al. 1979)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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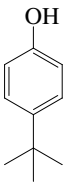
14.1.1.17 *p-tert*-Butylphenol



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: $C_{10}H_{14}O$, $(CH_3)_3CC_6H_4OH$
Molecular Weight: 150.217
Melting Point (°C):
98 (Lide 2003)
Boiling Point (°C):
237 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
152.0 (20°C, Stephenson & Malanowski 1987)
192.2 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
9.90 (McLeese et al. 1979)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
67.33, 50.62 (25°C, bp, Dreisbach 1955)
50.54 (at normal boiling point, Handley et al. 1964)
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: 0.192 (mp at 98°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
650 (20–25°C, Geyer et al. 1981)
1000 (Thomas 1982)
700 (Verschueren 1983)
580 (Yalkowsky et al. 1987)
580 (shake flask-UV, Ahel & Giger 1993a)
1850 (shake flask-HPLC/UV at pH 6.05, Varhaníčková 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 (calculated-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., Weast 1972–73)
5.072 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 512.693/(T/K)] × 10^{0.834403 – 2.10918 × 10^{-4}·(T/K) + 0.554077 × 10^{-7}·(T/K)^2}; temp range 343.15–524.76 K (Cox eq., Chao et al. 1983)
1.24 (supercooled liquid P_L, extrapolated-Antoine eq., Boublik et al. 1984)

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log (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, Boublik et al. 1984)
1.25 (extrapolated-Antoine eq., Dean 1985)
log (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 (P_S/kPa) = 11.46945 – 4405.873/(T/K); temp range 280–304 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.13162 – 1632.939/(–117.258 + T/K), temp range: 471–525 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
log (P/Pa) = 122.26679 – 8003.926/(T/K) – 40.16380·log (T/K) + 1.40155×10^{-2}·(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 (P/mmHg) = –54.7404 – 2.4727×10^3/(T/K) + 28.991·log (T/K) – 3.9356×10^{-3}·(T/K) + 1.543×10^{-5}·$(T/K)^2$; temp range 372–734 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/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 χ, Nirmalakhandan & Speece 1988)

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

3.04 (shake flask, Geyer et al. 1984)
2.94, 3.14 (shake flask-OECD 1981 Guideline, 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, $t_{½}$:

Volatilization: volatilization

$t_{½}$ = 117 h from water body with depth of 1 m (Thomas 1982).

Half-Lives in the Environment:

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TABLE 14.1.1.17.1
Reported vapor pressures of *p-tert*-butylphenyl 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/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Handley et al. 1964			
summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.0	133.3	198.21	33059	mp/°C	99.55
99.2	666.6	204.527	39955	bp/°C	239.83
114	1333	209.901	46592	for temp range:	
129.5	2666	214.892	53489	198–251°C	
146	5333	219.142	59984	eq. 2	P/mmHg
156	7999	223.088	66579	A	6.99455
170.2	13332	226.818	73350	B	1623.046
191.5	26664	230.203	79963	C	154.716
214	53329	233.457	86724	ΔH_V/(kJ mol^{-1})	
238	101325	236.342	92123	at bp	50.54
		239.305	100052		
mp/°C	99.0	242.180	106758		
		244.560	113369		
		247.015	120049		
		249.336	126634		
		251.608	133354		

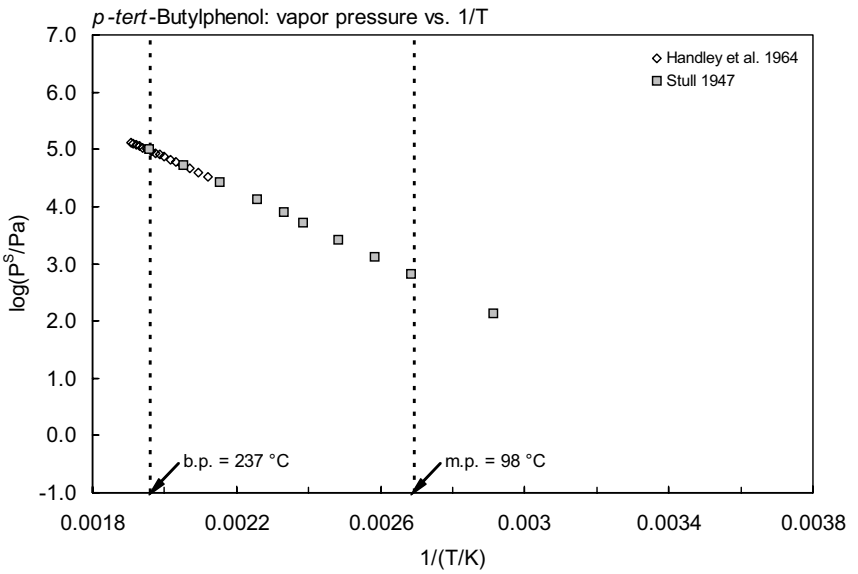

FIGURE 14.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for *p-tert*-butylphenol.

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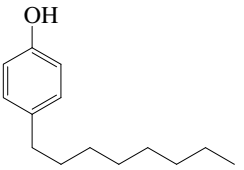
14.1.1.18 4-Octylphenol



Common Name: 4-Octylphenol
Synonym: *p*-octylphenol
Chemical Name: 4-octylphenol
CAS Registry No: 27193-28-8
Molecular Formula: $C_{14}H_{22}O$, $C_8H_{17}C_6H_4OH$
Molecular Weight: 206.324
Melting Point (°C):
43 (Lide 2003)
Boiling Point (°C):
280-283 (Lewis 1996)
Density (g/cm^3 at 20°C):
0.941 (at 24°C, Lewis 1996)
Molar Volume (cm^3/mol):
281.0 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.666 (mp at 43°C)

Water Solubility (g/m^3 or mg/L at 25°C):
12.6 ± 0.50 (generator column-HPLC/fluo., Ahel & Giger 1993a)
14.1 ± 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 m^3/mol at 25°C):
0.4916 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
3.70 (calculated-π substituent const. or fragment const., McLeese et al. 1981)
4.12 ± 0.10 (shake flask-HPLC/fluo., Ahel & Giger 1993b)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: average exptl. rate constant k = 0.0894 h^{-1} compared to group contribution method predicted rate constants k = 0.1124 h^{-1} (nonlinear) and k = 0.0982 h^{-1} (Tabak & Govind 1993).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

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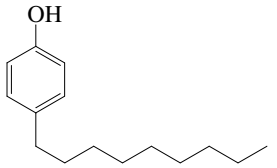
14.1.1.19 4-Nonylphenol



Common Name: 4-Nonylphenol
Synonym: *p*-nonylphenol
Chemical Name: 4-nonylphenol
CAS Registry No: 104-40-5; 25154-52-3
Molecular Formula: $C_{15}H_{24}O$, $C_9H_{19}C_6H_4OH$
Molecular Weight: 220.351
Melting Point (°C):
42 (Lide 2003
Boiling Point (°C):
approx. 295 (Lide 2003)
Density (g/cm^3 at 20°C):
1.513 (Budavari 1989)
Molar Volume (cm^3/mol):
231.1 (20°C, Stephenson & Malanowski 1987)
303.2 (calculated-Le Bas method at normal boiling)
Acid Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.681 (mp at 42°C)

Water Solubility (g/m^3 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)
log (P_L/kPa) = 6.87147 – 2547.289/(–67.246 + T/K), temp range 487–595 K (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 m^3/mol at 25°C):
1.5705 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
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, Itokawa et al. 1989)
4.48 ± 0.12 (shake flask-HPLC/fluo., Ahel & Giger 1993b)
6.36 (calculated-CLOGP 3.51, Jaworska & Schultz 1993)

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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, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: average exptl. 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: $t_{½}$ = 4 d in salmon before excretion (McLeese et al. 1981).

TABLE 14.1.1.19.1
Reported vapor pressures of 4-nonylphenol at various temperatures

Hon et al. 1976	
ebulliometry	
t/°C	P/Pa
214.78	6557
251.33	19998
261.87	26679
274.76	37250
283.74	46663
289.28	53364
298.78	66656
303.76	74873
307.72	81628
310.82	87441
314.17	94271
317.1	100170
321.81	110655
bp/°C	317.61

(Continued)

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TABLE 14.1.1.19.1 *(Continued)*

Hon et al. 1976	
ebulliometry	
t/°C	**P/Pa**
$\log P = A - B/(C + t/°C)$	
	P/mmHg
A	7.74950
B	2550.67
C	260.28
$\Delta H_V/(kJ\ mol^{-1})$	
at bp	61.923

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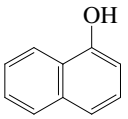
14.1.1.20 1-Naphthol



Common Name: 1-Naphthol
Synonym: α-naphthol, 1-naphthalenol, 1-hydroxynaphthalene
Chemical Name: 1-naphthol
CAS Registry No: 90-15-3
Molecular Formula: $C_{10}H_8O$, $C_{10}H_7OH$
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/cm^3):
1.0989 (99°C, Weast 1982–83)
1.0954 (99°C, Dean 1985)
Acid Dissociation Constant, pK_a:
9.20 (McLeese et al. 1979)
9.30 (Dean 1985)
Molar Volume (cm^3/mol):
131.2 (99°C, Stephenson & Malanowski 1987)
155.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.47 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
63.6 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.206 (mp at 95°C)

Water Solubility (g/m^3 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, Vonterres 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 Vonterres 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 (P_S/kPa) = 12.20753 – 4873.394/(T/K); temp range 298–312 K (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = 10.70115 – 4405.522/(T/K); temp range 314–324 K (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)
log (P_L/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·m^3/mol at 25°C):
0.49 (calculated-P/C, this work)

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

2.98	(shake flask-UV, Hansch & Anderson 1967)
2.98, 2.84, 2.31	(Hansch & Leo 1979)
2.28	(HPLC-k′ correlation, Haky & Young 1984)
2.84	(recommended, Sangster 1989, 1993)
2.84	(CPC centrifugal partition chromatography, Gluck & Martin 1990)
3.13	(back-flushing-CPC centrifugal partition chromatography, Menges et al. 1990)
2.81	(shake flask-HPLC, Menges et al. 1991)
3.02	(concurrent chromatography, Berthod et al. 1988)
2.84	(COMPUTOX, Kaiser 1993)
2.43	(HPLC-RT correlation, Ritter et al. 1994)
2.84	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.64	(soil and sediment, Hassett et al. 1981)
3.33	(soil, Means et al. 1982)
3.41	(soil, calculated-MCI χ, Sabljic 1987)
2.10–2.77	(soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987)
2.63–2.99	(soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987)
1.84–2.1	(soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987)
1.99–2.66	(soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987)
1.30–1.90	(soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987)
2.89	(soil, calculated-MCI χ, Bahnick & Doucette 1988)
2.52–2.96, 2.53	(soil: quoted, calculated-K_{OW}, Xing et al. 1994)
1.92–2.64	(organic sorbent: cellulose, lignin, Xing et al. 1994)
3.31, 2.91, 2.61	(RP-HPLC-k′ correlation on 3 different stationary phases, Szabo et al. 1995)
2.61; 3.48	(HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)

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

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation: average rate of biodegradation 38.4 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).
Biotransformation:
Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

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TABLE 14.1.1.20.1
Reported vapor pressures of 1-naphthol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
94.0	133.3	141.5	1333
125.5	666.6	164.8	3333
142	1333	184.2	6666
158	2666	196.9	9999
177.8	5333	206.0	13332
190	7999	219.3	19998
206	13332	229.0	26664
229.6	26664	236.4	33330
255.8	53329	244.0	39997
282.5	101325	246.5	43330
		250.2	46663
mp/°C	96.0	255.1	53329
		260.3	59995
		264.8	66661
		265.7	73327
		272.0	79993
		275.2	86659
		278.3	93325
		282.5	101325

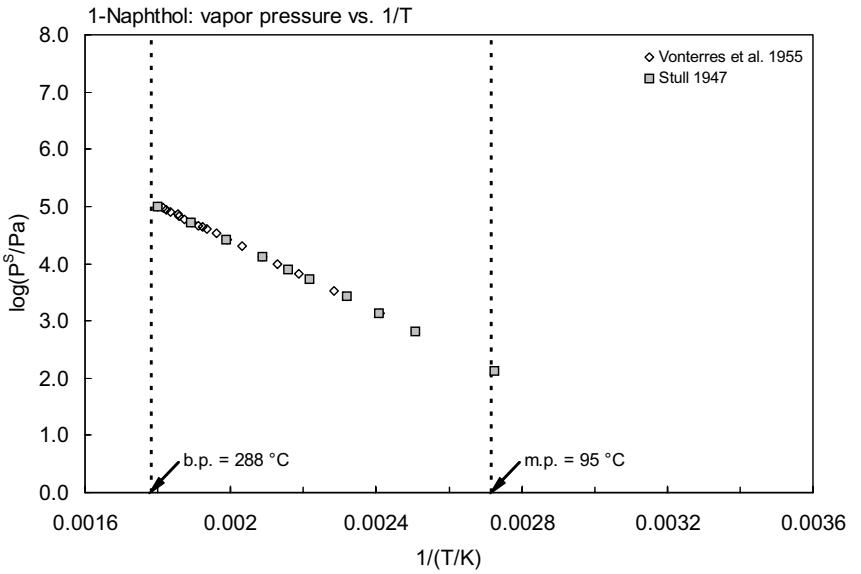

FIGURE 14.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for 1-naphthol.

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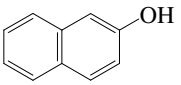
14.1.1.21 2-Naphthol



Common Name: 2-Naphthol
Synonym: β-naphthol, 2-naphthalenol, 2-hydroxynaphthalene
Chemical Name: 2-naphthol
CAS Registry No: 135-19-3
Molecular Formula: $C_{10}H_7OH$
Molecular Weight: 144.170
Melting Point (°C):
121.5 (Lide 2003)
Boiling Point (°C):
285 (Lide 2003)
Density (g/cm^3 at 20°C):
1.280 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
9.57 (Dean 1985)
Molar Volume (cm^3/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/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):
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°, Stull 1947)
1333* (144.0°C, ebulliometry, measured range 144.0–288.0°C, Vonterres 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 Vonterres 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_S/kPa) = 12.48704 – 5110.333/(T/K), temp range 298–312 K (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = 10.80636 – 4586.029/(T/K), temp range 314–332 K (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = 9.273 – 4112/(T/K), temp range 283–323 K (Antoine eq.-III, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.22927 – 2827.5/(–19.868 + T/K), temp range 401–561 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

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

0.280 (calculated-P/C, this work)

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

2.84	(shake flask-UV, Hansch & Anderson 1967)
2.70, 2.84, 2.89	(Hansch & Leo 1979)
2.01, 2.46	(HPLC-k′ correlation, Eadsforth 1986)
2.84	(recommended, Sangster 1989)
2.85	(centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
2.70	(EPA CLOGP Data Base, Hulzebos et al. 1993)
2.70	(COMPUTOX, Kaiser 1993)
2.70	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.33	(soil, Means et al. 1982)
3.41	(soil, calculated-MCI χ, Sabljic 1987)
2.10–2.77	(soil, calculated-K_{OW} based on model of Karickhoff et al. 1979, Sabljic 1987)
2.63–2.99	(soil, calculated-K_{OW} based on model of Kenaga & Goring 1980, Sabljic 1987)
1.84–2.19	(soil, calculated-K_{OW} based on model of Briggs 1981, Sabljic 1987)
1.99–2.66	(soil, calculated-K_{OW} based on model of Means et al. 1982, Sabljic 1987)
1.30–1.90	(soil, calculated-K_{OW} based on model of Chiou et al. 1983, Sabljic 1987)

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

Volatilization:
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:

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TABLE 14.1.1.21.1
Reported aqueous solubilities and vapor pressures of 2-naphthol at various temperatures

Aqueous solubility				Vapor pressure			
McCune & Wilhelm 1949		Moyle & Tyner 1953		Stull 1947		Vonterres et al. 1955	
shake flask		shake flask-UV spec.		summary of literature data		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
15.55	501	6.90	355	128.6	666.6	144.0	1333
16.24	526	13.45	487	145.5	1333	158.0	3333
23.20	680	17.7	561	161.8	2666	188.0	6666
31.25	928	21.5	713	181.7	5333	200.5	9999
		29.5	876	193.7	7999	210.0	13332
log (100·C_W) = A – B/(T/K)		33.3	985	209.8	13332	223.1	19998
C_W	g/100 mL	38.7	1304	234.0	26664	233.0	26664
A	5.8833	44.5	1609	260.6	53329	246.0	33330
B	1495.84	48.5	2001	288.0	101325	247.4	39997
		55.2	2460			251.0	43330
		60.0	3034	mp/°C	122.5	254.2	46663
		68.1	4222			260.2	53329
		75.0	5493			265.1	59995
						269.0	66661
						273.0	73327
						276.6	79993
						279.7	86659
						283.0	93325
						288.0	101325

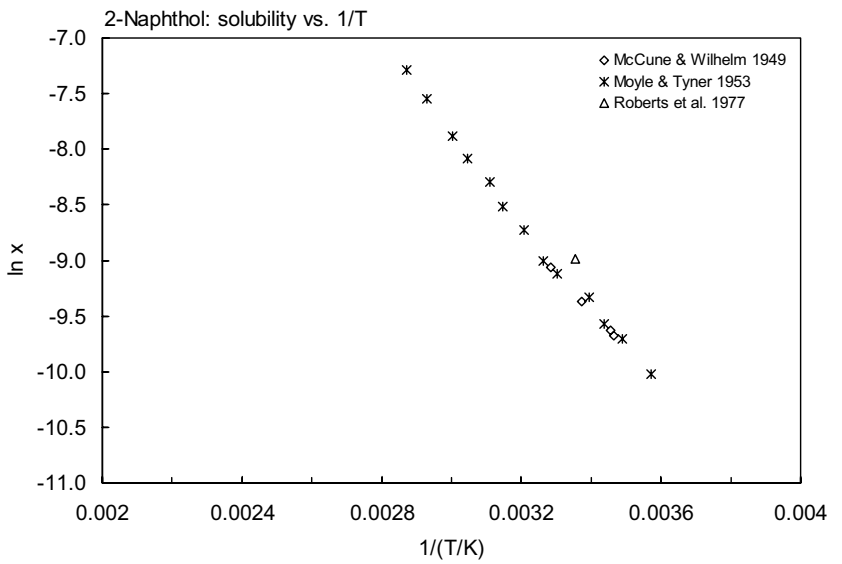

FIGURE 14.1.1.21.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-naphthol.

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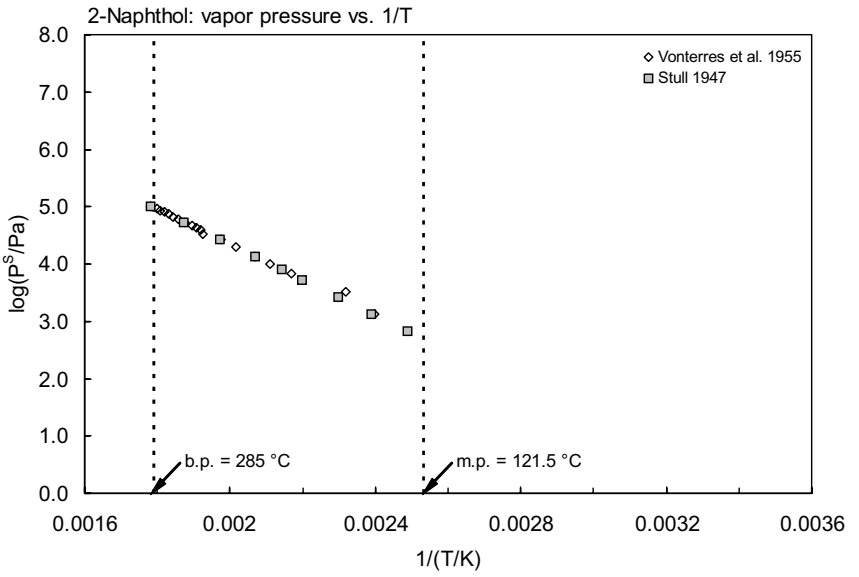

FIGURE 14.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for 2-naphthol.

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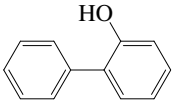
14.1.1.22 2-Phenylphenol (2-Hydroxybiphenyl)



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: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$
Molecular Weight: 170.206
Melting Point (°C):
57.5 (Weast 1982–83)
Boiling Point (°C):
286 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.213 (Dean 1985)
1.200 (25°C, Verschueren 1983)
Molar Volume (cm^3/mol):
192.0 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
9.55 (Dean 1985)
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: 0.480 (mp at 57.5°C)

Water Solubility (g/m^3 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, Vonterres 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/(72.282 + t/°C), temp range 161.9–275°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
30.0 (interpolated-Antoine eq.-I, solid P_S, Stephenson & Malanowski 1987)
log (P_S/kPa) = 10.8635 – 4326.754/(T/K), temp range 291–314 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/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·m^3/mol at 25°C):

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

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Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{½}$ = 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 $t_{½}$ = 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);

$t_{½}$(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); $t_{½}$(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 $t_{½}$ = 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 $t_{½}$ = 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; Güesten et al. 1981; quoted, Howard et al. 1991); $t_{½}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater:$t_{½}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 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

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
100	133.3	161.9	1333
131.6	666.6	168.0	3333
146.2	1333	188.1	6666
163.3	2666	198.0	9999
180.3	5333	206.8	13332
192.2	7999	219.0	19998
205.9	13332	228.1	26664
227.9	26664	235.2	33330
251.8	53329	241.6	39997
275.0	101325	244.0	43330
		247.4	46663

(Continued)

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TABLE 14.1.1.22.1 *(Continued)*

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
mp/°C	56.6	252.0	53329
		257.0	59995
		261.0	66661
		264.0	73327
		268.0	79993
		270.0	86659
		273.8	93325
		275.0	101325
		bp/°C	278.004

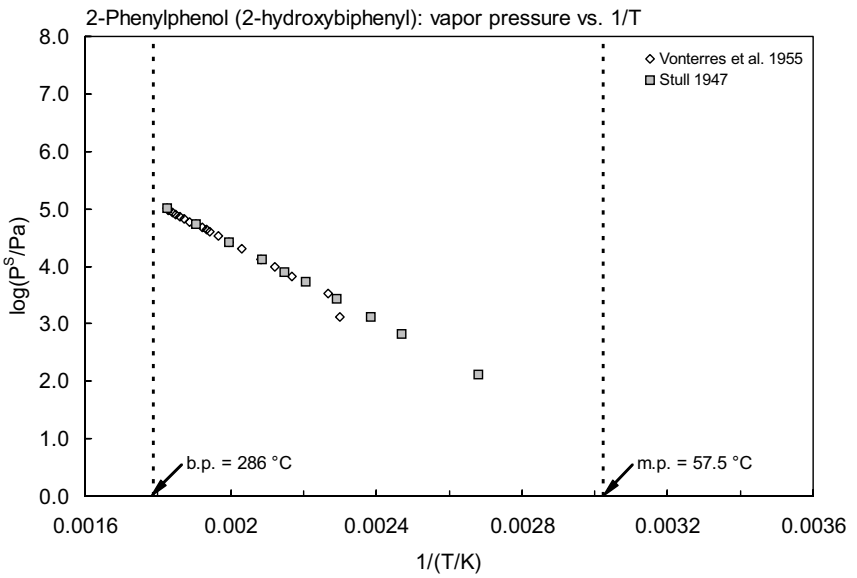

FIGURE 14.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 2-phenylphenol.

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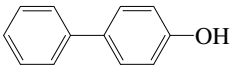
14.1.1.23 4-Phenylphenol (4-Hydroxybiphenyl)



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: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$
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/cm^3 at 20°C):
Molar Volume (cm^3/mol):
192.0 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
9.55 (Dean 1985)
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: 0.0414 (mp at 166°C)

Water Solubility (g/m^3 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):
1333* (176.2°C, summary of literature data, temp range 176.2–308°C, Stull 1947)
1333* (177.0°C, ebulliometry, measured range 177.0–308.0°C, Vonterres et al. 1955)
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)] × 10^{0.949514 – 5.554686 × 10^{-4}·(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 Vonterres et al. 1955, Boublik et al. 1984)
0.020 (extrapolated-Antoine eq., Dean 1985)
log (P/mmHg) = 8.6575 – 3022.8/(216.1 + t/°C); temp range:177–308°C (Antoine eq., Dean 1985, 1992)
0.00153 (extrapolated-Antoine eq., solid P_S, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.17513 – 5066.004/(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 m^3/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)

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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, $t_{½}$:

Half-Lives in the Environment:

TABLE 14.1.1.23.1
Reported vapor pressures of 4-phenylphenol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
176.2	1333	177.0	1333
193.8	2666	199.2	3333
213.0	5333	217.8	6666
225.3	7999	229.0	9999
240.9	13332	237.4	13332
263.2	26664	250.0	19998
285.5	53329	260.2	26664
308.0	101325	267.1	33330
		273.8	39997
mp/°C	164.5	276.0	43330
		278.8	46663
		283.0	53329
		287.1	59995
		291.0	66661
		294.7	73327
		297.8	79993
		300.6	86659
		303.5	93325
		308.0	101325
		bp/°C	307.194

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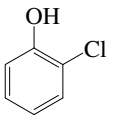
14.1.2 CHLOROPHENOLS

14.1.2.1 2-Chlorophenol



Common Name: 2-Chlorophenol
Synonym: *o*-chlorophenol, 1-chloro-2-hydroxybenzene
Chemical Name: 2-chlorophenol
CAS Registry No: 95-57-8
Molecular Formula: $C_6H_4(OH)Cl$
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^3):
1.2634 (20°C, Weast 1982–83)
1.257 (25°C, Krijgsheld & van der Gen 1986)
Acid Dissociation Constant, pK_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^3/mol):
101.8 (20°C, Stephenson & Malanowski 1987)
124.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
40.05, 49.25 (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
13.50 (Dreisbach 1955)
10.75 (Tsonopoulos & Prausnitz 1971)
12.52 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
38.12 (Tsonopoulos & Prausnitz 1971)
44.24 (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. 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)

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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):

316* (interpolated-regression of tabulated data, temp range 12.7–174.5°C, Stull 1947)
208 (calculated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.05272 – 1589.1/(206.0 + t/°C), temp range 80–300°C (Antoine eq. for liquid state, Dreisbach 1955)
313 (extrapolated from Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 10341.1/(T/K)] + 7.952334; temp range 12.1–174.5°C (Antoine eq., Weast 1972–73)
5532 (80°C, Verschueren 1977, 1983)
293, 180.7 (extrapolated, Antoine eq., Dean 1985)
log (P/mmHg) = 6.87731 – 1471.61/(193.17 + t/°C); temp range 80–200°C (Antoine eq., Dean 1985, 1992)
131.8 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.78693 – 1314.9/(–101.95 + T/K), temp range 333–449 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.3685 – 1096.98/(–122.58 + T/K); temp range 354–448 K (Antoine eq.-II, Stephenson & Malanowski 1987)
737, 1329, 2278, 3736, 5907 (50, 60.24, 69.94, 79.95, 89.94°C, calculated-Antoine eq. of Stephenson & Malanowski 1987, Tabai et al. 1997)

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

1.065 (calculated-P/C, Mabey et al. 1982)
0.688 (calculated-P/C, Shiu et al. 1994)
0.661 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
k_H/kPa = 161.250 – 12658.0/(T/K) – 20.4027; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

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

2.15 (shake flask-UV, Fujita et al. 1964;)
2.15, 2.19 (Leo et al. 1971)
2.20 (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)
2.12 (20°C, shake flask, Korenman 1974)
2.15 (LC-k′ correlation, Carson et al. 1975)
2.17 (Hansch & Leo 1979)
2.16 (shake flask-LSC, Banerjee et al. 1980)
0.83 (RP-HPLC-RT correlation, Veith et al. 1980)
2.11 (RP-HPLC-RT correlation, Butte et al. 1981)
2.03 (shake flask, Dearden & Bresnen 1981)
2.16 ± 0.03 (HPLC-k′ correlation, Hammers et al. 1982)
2.32 (RP-HPLC-RT correlation, Chin et al. 1986)
1.56, 1.99 (HPLC-k′ correlation, Eadsforth 1986)
2.09 (HPLC-RT correlation, Miyake et al. 1986)
2.13 (shake flask-UV, Miyake et al. 1987)
2.16 (shake flask-CPC, Berthod et al. 1988)
2.24 (batch equilibration-UV, Beltrame et al. 1988)
2.11 (centrifugal partition chromatography, Gluck & Martin 1990)
2.25 (back flashing-CPC centrifugal partition chromatography; Menges et al. 1990)
2.05 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
2.17 (counter-current chromatography, Berthod et al. 1992)
2.15 (recommended, Sangster 1993)
2.29 (shake flask-GC, Kishino & Kobayashi 1994)
2.15 (recommended, Hansch et al. 1995)

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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_{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_{OW}, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

3.70, 3.60 (sediment: fine, coarse; Isaacson & Frink 1984)
1.86 (sediment-water, calculated-K_{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_{OW}, Howard 1989)
1.82 (calculated-K_{OW}, Kollig 1993)
2.60 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization: $t_{½}$ = 1.35, 1.60 h from stirred and static water at 23.8°C (Chiou et al. 1980; Howard 1989);
$t_{½}$ = 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 $t_{½}$ = 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_{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:
$k(aq.) < 7 \times 10^5$ M^{-1} h^{-1} for singlet oxygen and 1×10^7 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)
$k(aq.) = 66 \times 10^6$ M^{-1} s^{-1} at pH 8, $k = (1.1 \pm 0.3) \times 10^3$ M^{-1} s^{-1} for non-protonated species, $k = (0.2 \pm 0.1) \times 10^9$ M^{-1} s^{-1} for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.8–4 and 20–23°C (Hoigné & Bader 1983b)
$k_{OH} = 1.3 \times 10^{-11}$ cm^3 molecule s^{-1} for reaction with OH radical in air (Bunce et al. 1991)
$k(aq.) = (9.2 \pm 9.4) \times 10^6$ M^{-1} 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 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 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 exptl. conditions (Baker et al. 1980);
rate constants k = 1.0 d^{-1} with $t_{½}$ = 0.7 d in adopted activated sludge and k = 0.3 d^{-1} with $t_{½}$ = 2.3 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 -mol L^{-1} d^{-1} in freshwater and k = 8 -mol L^{-1} d^{-1} in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990).

Biotransformation: rate constant for bacterial transformation of 1×10^{-7} mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982);
microbial transformation $k = (7.1 \pm 1.6) \times 10^{-11}$ L $organism^{-1}$ h^{-1} (Paris et al. 1983; quoted, Steen 1991);
degradation $k = 3.49 \times 10^{-17}$ (± 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:

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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: $t_{½}$ = 16.8 d in sludge and $t_{½}$ = 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 = 3.01×10^{-2} min^{-1} in the absence of DOM at 313 nm (Kawaguchi 1992).

Groundwater:

Sediment:

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)

$t_{½}$ = 51 d in a coarse sandy soil, $t_{½}$ = 110 d in sandy loam (Kjeldsen et al. 1990)

$t_{½}$ = 7.2 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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: $t_{½}$ < 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

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922		Achard et al. 1996		Stull 1947	
synthetic method		shake flask-conductimetry		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa
–0.20	15600	15.4	24007	12.1	133.3
–0.30	24400	24.6	22660	38.2	666.6
82.9	37600	34.5	24007	51.2	1333
106.3	51200			65.9	2666
159.1	135800			82.0	5333
165.8	169500			92.0	7999
170.7	225900			106.0	13332
173.0	330000			126.4	26664
172.9	450400			149.8	53329
170.1	549500			174.5	101325
166.2	607200				
156.6	706200			mp/°C	7.0
118.9	828200				
91.5	859000				
–2.0	877300				
–4.0	892500				
–5.0	896200				
–8.0	908700				
–8.2	922000				
–6.0	929200				
–1.50	967900				
2.0	983900				
7.0	1000000				
critical solution temp 173°C					

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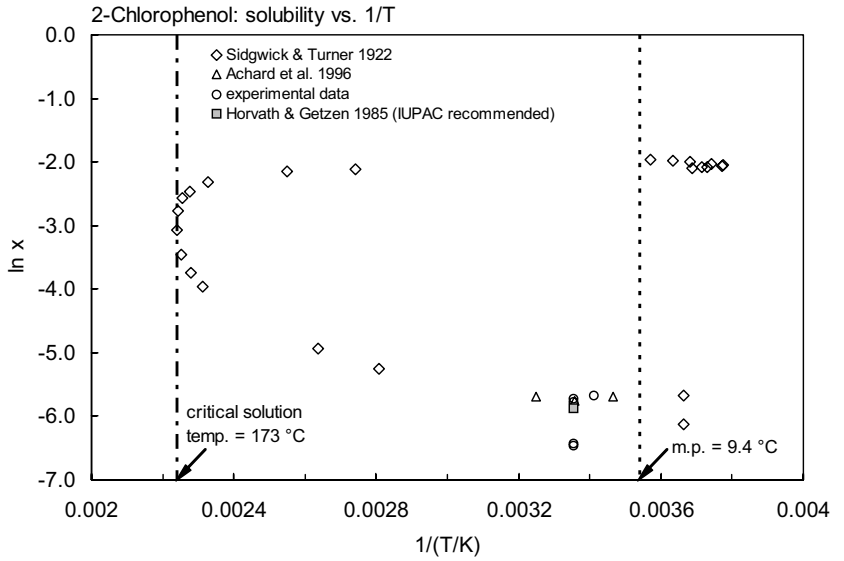

FIGURE 14.1.2.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-chlorophenol.

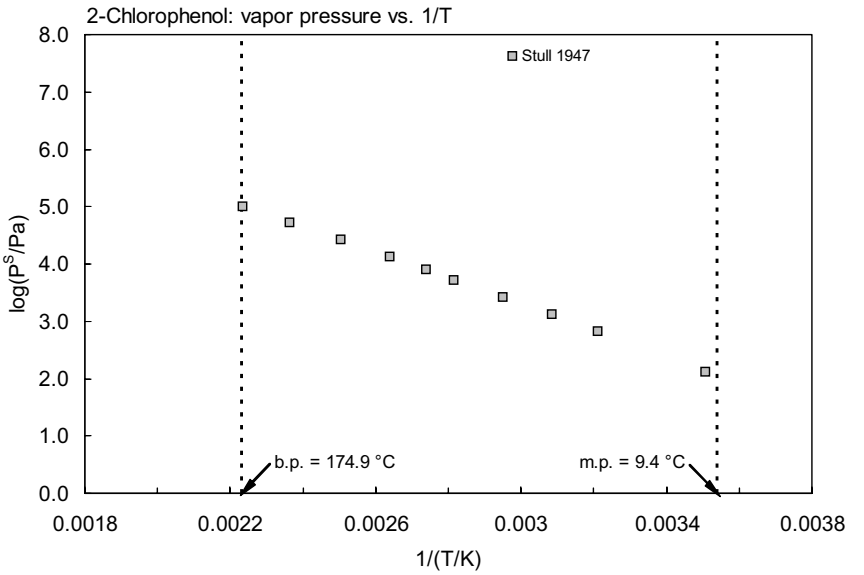

FIGURE 14.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-chlorophenol.

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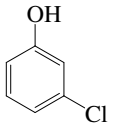
14.1.2.2 3-Chlorophenol



Common Name: 3-Chlorophenol
Synonym: *m*-chlorophenol, 1-chloro-3-hydroxybenzene
Chemical Name: 3-chlorophenol
CAS Registry No: 108-43-0
Molecular Formula: C_6H_4ClOH
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/cm^3, 20°C):
1.268 (25°C, Weast 1982–83)
Acid Dissociation Constant, pK_a:
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)
9.12 (Serjeant & Dempsey 1979; Howard 1989; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)
8.97 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Renner 1990; Ma et al. 1993)
9.10 (Dean 1985; Schultz & Cajina-Quezada 1987)
9.02 (Krijgsheld & van der Gen 1986)
9.37 (quoted from Ugland et al. 1981, Lagas 1988)
Molar Volume (cm^3/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 (exptl.; 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/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):
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)

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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·m^3/mol):
0.0567 (calculated, Hine & Mookerjee 1975)
0.2045 (calculated-P/C, Shiu et al. 1994)
k_H/kPa = 22.0921 – 6444.46/(T/K); temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

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-π 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. fetida 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 $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization: estimated $t_{½}$ ~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 $t_{½}$ = 1.96 d (Howard 1989);
measured pseudo-first-order reaction k = 0.048 ± 0.001 min^{-1} for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

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Oxidation: rate constant k = (5.4 ± 1.0) × 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).
Bioconcentration 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: $t_{½}$ = (14.5 ± 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 $t_{½}$ = 2.5 d from Kooyenburg soil, $t_{½}$ = 5.4 d from Holten soil with earthworms *e. fetida andrei* and $t_{½}$ = 2.6 d from Kooyenburg soil, $t_{½}$ = 2.1 d from Holten soil with earthworms *l. rubblus* (van Gestel & Ma 1988);
$t_{½}$ = 15.1 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922				Stull 1947	
synthetic method				summary of literature data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa
–0.18	7300	3.2	844700	44.2	133.3
1.20	12500	–0.90	-*	72.0	666.6
2.5	18500	4.5	871900	86.1	1333
82.25	51200	–4.8	886600*	101.7	2666
118.0	111300	–8.2	901100*	118.0	5333
123.0	135600	–13.2	917300*	129.4	7999
127.5	178400	10.8	922300	143.0	13332
130.8	320200	–17.0	-*	164.8	26664
130.7	388900	17.0	951000	188.7	53329
130.5	461200	22.2	971100	214.0	101325
129.1	536500	32.5	1000000		
109.8	712300			mp/°C	32.5
23.1	823000	critical solution temp 130.8°C			
11.8	829000	*metastable point			

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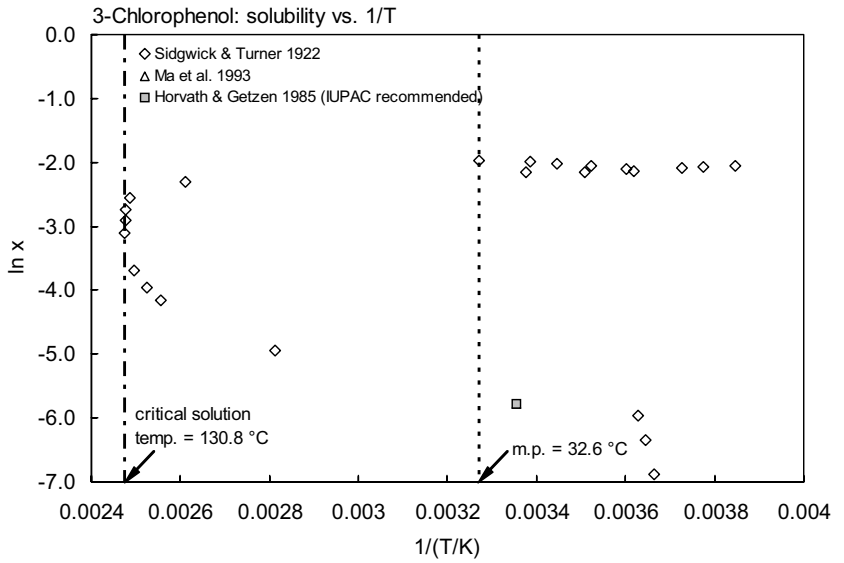

FIGURE 14.1.2.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 3-chlorophenol.

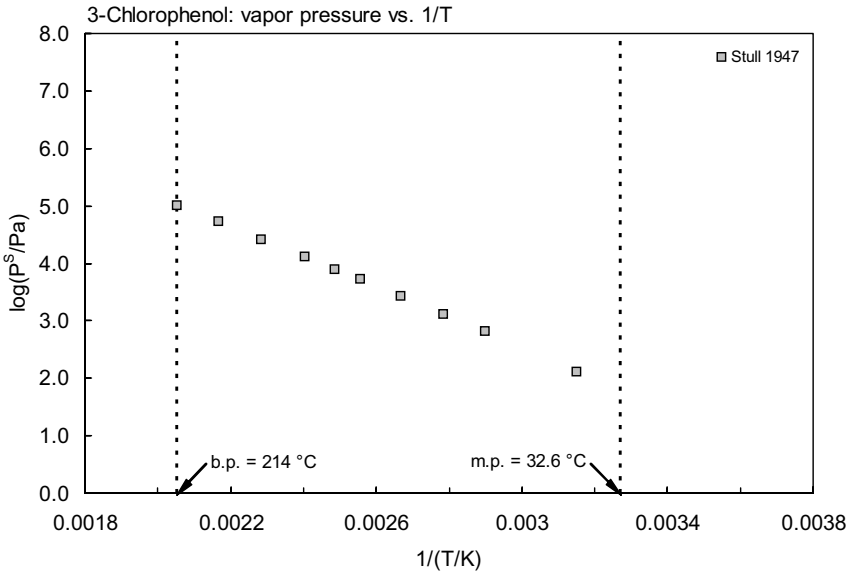

FIGURE 14.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorophenol.

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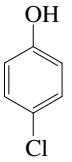
14.1.2.3 4-Chlorophenol



Common Name: 4-chlorophenol
Synonym: *p*-chlorophenol, 1-chloro-4-hydroxybenzene
Chemical Name: 4-chlorophenol
CAS Registry No: 106-48-9
Molecular Formula: ClC_6H_4OH
Molecular Weight: 128.556
Melting Point (°C):
42.8 (Lide 2003)
Boiling Point (°C):
220 (Lide 2003)
Density (g/cm^3 at 20°C):
1.2651 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
9.37 (Farquharson et al. 1958; Ugland et al. 1981; Saarikoski & Viluksela 1982; Renner 1990)
9.18 (Doedens 1967)
9.42 (Pearce & Simkins 1968)
9.14 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988; Argese et al. 1999)
9.41 (Serjeant & Dempsey 1979)
9.38 (Paris et al. 1982; Krijgsheld & van der Gen 1986)
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 (cm^3/mol):
101.6 (40°C, Stephenson & Malanowski 1987)
124.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
14.69 (Tsonopoulos & Prausnitz 1971)
14.07; 16.2 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
46.44 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25° C (assuming ΔS_{fus} = 56 J/mol K), F: 0.669 (mp at 42.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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, Achard et al. 1996)
20712* (11.05°C, shake flask-optical method, measured range 282.2–386.1 K, Jaoui et al. 1999)
25519* (24.85°C, shake flask-optical method, measured range 298–341.9 K, Jaoui et al. 2002)
ln [S/(mol kg^{-1})] = 5.6451 – 716.81/(T/K); temp range 282–342 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

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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)
13.3, 33.3 (20°C, 30°C, Verschueren 1977, 1983)
3.47 (extrapolated liquid value, Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 8.83238 – 1385.1/(–131.1 + T/K), temp range 373–493 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/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)
k_H/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, Mirrlees 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, electrometric 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)
2.377, 2.686, 2.025, 2.222, 2.332 (soils, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
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)

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

Volatilization: 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); $t_{½}$ = 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 $t_{½}$ = 63 h for distilled water in summer (mean temp 25°C) and k = 0.007 h^{-1} with $t_{½}$ = 99 h in winter (mean temp 14°C); k = 0.03 h^{-1} with $t_{½}$ = 28 h for estuarine water in summer and k = 0.011 h^{-1} with $t_{½}$ = 63 h in winter exposed to full sunlight and microbes (Hwang et al. 1986)

photo-mineralization rate constants: k = 0.012 h^{-1} with $t_{½}$ = 58 d for distilled water in summer and k = 0.003 h^{-1} with $t_{½}$ = 224 d in winter; k = 0.07 h^{-1} with $t_{½}$ = 10 d in summer and k = 0.007 h^{-1} with $t_{½}$ = 95 d in winter for surface estuarine water exposed to full sunlight and microbes (Hwang et al. 1986);

photo-degradation k = 564×10^3 min^{-1} with $t_{½}$ = 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_{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.) = (600 ± 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(aq.) = 34×10^6 M^{-1} s^{-1} at pH 8, and k = (600 ± 100) M^{-1} s^{-1} for non-protonated species, k = $(0.6 \pm 0.2) \times 10^9$ M^{-1} s^{-1} for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.5–6 and 20–23°C (Hoigné & Bader 1983b)

k(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 = 1877×10^3 min^{-1} with a half-life of 0.4 min for reaction with Fenton's reagent; k_{O3} = 17×10^3 min^{-1} with a half-life of 38.15 min at pH 2; and k_{O3} = 239×10^3 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);

$t_{½}$ = 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);

$t_{½}$ = 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 $t_{½}$ = 11 h for estuarine water in summer and $t_{½}$ = 0.006 h^{-1} with $t_{½}$ = 116 h in winter in the darkness (Hwang et al. 1986)

mineralization k = 0.293 h^{-1} with $t_{½}$ = 2 d for estuarine water in summer and k = 0.003 h^{-1} with $t_{½}$ = 231 d in winter in the darkness (Hwang et al. 1986); degradation rate constants k = 0.035 d^{-1} with $t_{½}$ = 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 µmol L^{-1} d^{-1} in freshwater and 22 µmol L^{-1} d^{-1} in saline water with acclimated sulfindogenic sediment cultures (Häggblom & Young 1990);

average transformation rate of 53 µmol 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).

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Biotransformation: microbial transformation rate constant of $(1.7 \pm 0.9) \times 10^{-12}$ L organism^{-1} h^{-1} (Paris et al. 1982); microbial transformation rate constant of $(4.7 \pm 1.6 \times 10^{-11}$ L organism^{-1} h^{-1} to $(9.0 \pm 1.7) \times 10^{-11}$ L organism^{-1} h^{-1} in pond and river samples at five different sites (Paris et al. 1983);
degradation rate k = 5.44×10^{-17} (± 32% SD) mol cell^{-1} h^{-1} from pure culture studies and 0.3×10^{-12} 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: $t_{½}$ = 1.96 d in the atmosphere (Howard 1989)
Surface water: $t_{½}$ = 475 h for biodegradation in river waters with a calculated first-order rate constant of 0.035 d^{-1} (Lee & Ryan 1979; quoted, Battersby 1990);
$t_{½}$ = 216–624 h and 72–1080 h for 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);
rate constant k = 600 ± 100 M^{-1} s^{-1} for the reaction with ozone at pH 1.5–6.0 (Hoigné & Bader 1983);
$t_{½}$ = 63 h in summer at season temp., 25°C, $t_{½}$ = 99 h in winter at season temp., 14°C in distilled water and 28 h in summer, $t_{½}$ = 63 h in winter in estuary surface water, based on photo-transformation rate (Hwang et al. 1986);
$t_{½}$ = 58 d in summer, $t_{½}$ = 224 d in winter in distilled water; and $t_{½}$ = 10 d in summer, $t_{½}$ = 95 d in winter in surface estuarine water, based on photo-mineralization rate (Hwang et al. 1986);
$t_{½}$ = 216 h at 21°C in Skidway River water (Pritchard 1987);
$t_{½}$ = 20 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 $t_{½}$ = 0.4 min for reaction with Fenton's reagent; $t_{½}$ = 38.15 min at pH 2, and $t_{½}$ = 3.4 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).
Ground water:
Sediment: $t_{½}$ = 72 h at 22°C in Skidway River water-sediment slurry (Pritchard 1987);
$t_{½}$ = 3 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)
$t_{½}$ = 2.5 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 1.0 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

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}	T/K	S/g·m^{-3}
–0.20	20700	15.1	23337	282.2	17856.	298.0	25519
65.0	39100	25.2	25540	284.2	20712	305.2	27010
113.8	106600	34.6	28499	308.3	27855	315.3	29389
125.0	205000			311.2	29283	319.7	30057
128.2	291600			324.2	32140	323.8	30919
128.7	425700			341.9	35711	332.7	32809
125.8	534900			354.7	41425	341.2	34608
122.4	596200			359.9	44282	298.0	25519
115.5	650500			362.7	48567	305.2	27010
107.7	693600			364.4	52852	315.3	29132
97.0	740300			365.7	54261	332.7	32809

(Continued)

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TABLE 14.1.2.3.1 *(Continued)*

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}	T/K	S/g·m^{-3}
35.5	840200			366.7	57852	339.5	34248
17.0	854200			386.1	117132	298.3	25583
5.5	861900					309.3	27872
0.5	889200					315.8	29235
6.2	924800					324.8	31124
11.0	944800					329.0	32024
14.2	957000					341.9	34763
18.0	968200						
19.5	972900					*some data from Achard et al. 1996, Jaoui et al. 1999	
41.0	1000000						
critical solution temp 129°C							
triple point –0.30°							

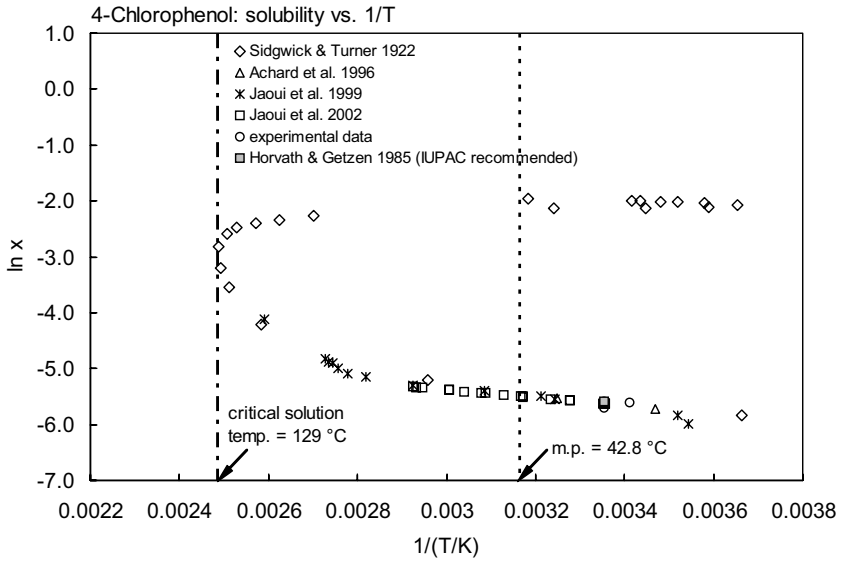

FIGURE 14.1.2.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chlorophenol.

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TABLE 14.1.2.3.2
Reported vapor pressures of 4-chlorophenol at various temperatures

Stull 1947	
summary of literature data	
t/°C	**P/Pa**
49.8	133.3
78.2	666.6
92.2	1333
108.1	2666
125.0	5333
136.1	7999
150.0	13332
172.0	26664
196.0	53329
220.0	101325
mp/°C	42.0

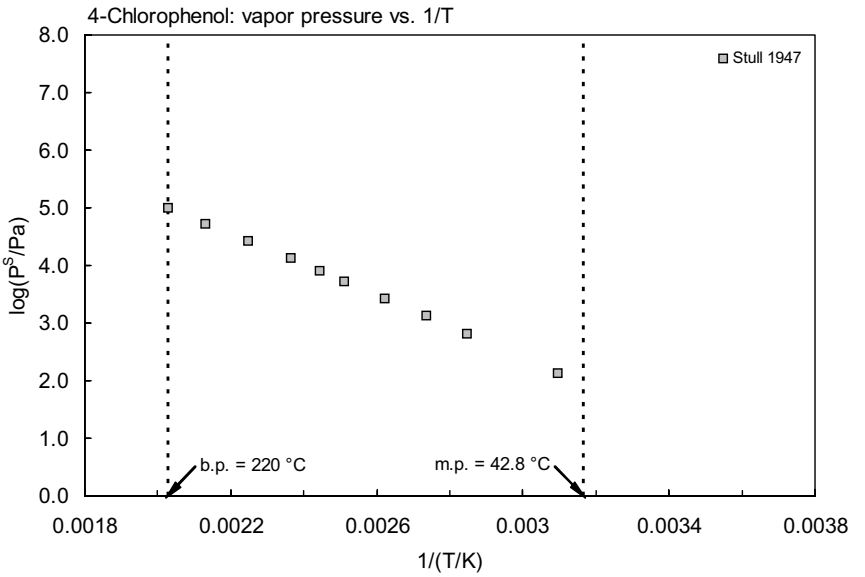

FIGURE 14.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorophenol.

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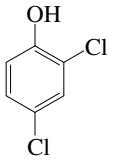
14.1.2.4 2,4-Dichlorophenol



Common Name: 2,4-Dichlorophenol
Synonym: 2,4-DCP
Chemical Name: 2,4-dichlorophenol
CAS Registry No: 120-83-2
Molecular Formula: $C_6H_4Cl_2O$, $C_6H_3Cl_2OH$
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/cm^3):
1.383 (at 60/25°C, Verschueren 1983)
Acid Dissociation Constant, pK_a:
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 (cm^3/mol):
145.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.09; 16.7 (exptl.; calculated-group additivity method, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus}= 56 J/mol K), F: 0.636 (mp at 45°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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)

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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/mmHg) = [–0.2185 × 13230.4/(T/K)] + 8.884810; 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_L/kPa) = 6.75941 – 1945.1/(–73.987 + T/K); temp range 326–483 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.32554 – 1807.32/(–69.17 + T/K); temp range 391–474 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/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/kPa = 24.9070 – 6791.07/(T/K); 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)
3.20, 3.17, 3.17 (20°C, shake flask-GC-calculated-regression, Xie & Dyrssen 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)

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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)
2.76 (soil, calculated-MCI χ, Sabljic 1987a,b)
2.49 (calculated-K_{OW}, Kollig 1993)
2.75 (soil, calculated-MCI $^1\chi$, 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)
2.609, 2.654, 2.460, 2.346, 2.540 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.49, 2.57, 2.77, 2.33 (soils: organic carbon OC -0.1% and pH 2.0–7.4, OC –0.1% and pH ≤ 5.8, OC –0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

photolysis:

$k_P = 0.82\ h^{-1}$ with $t_{½} = 0.8$ h for distilled water in summer at mean temp. 25°C, and $k_P = 0.21\ h^{-1}$ with $t_{½} = 3$ h in winter at mean temp. 11°C; $k_P = 1.16\ h^{-1}$ with $t_{½} = 0.6$ h for estuarine water in summer and $k_P = 0.44\ h^{-1}$ with $t_{½} = 2$ h in winter; $k_P = 1.0\ h^{-1}$ with $t_{½} = 0.7$ h in summer and $k_P = 0.38\ h^{-1}$ with $t_{½} = 2$ h in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-transformation, Hwang et al. 1986)

$k_P = 0.09\ h^{-1}$ with $t_{½} = 8$ d in summer and $k_P = 0.049\ h^{-1}$ with $t_{½} = 14$ d in winter for distilled water; $k_P = 0.20\ h^{-1}$ with $t_{½} = 4$ d in summer and $k_P = 0.04\ h^{-1}$ with $t_{½} = 17$ d in winter for estuarine water; $k_P = 0.12\ h^{-1}$ with $t_{½} = 6$ d in summer and $k_P = 0.05\ h^{-1}$ with $t_{½} = 14$ d in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-mineralization rate, Hwang et al. 1986)

photochemical-transformation $t_{½} = 2.5$–2.6 h in Xenotest 1200 (Svenson & Björndal 1988)

atmospheric and aqueous photolysis $t_{½} = 0.8$–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 $t_{½} = 17.5$ 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_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 7 \times 10^5\ M^{-1}\ h^{-1}$ for singlet oxygen, and $1 \times 10^7\ M^{-1}\ h^{-1}$ for peroxy 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, $k = 76 \times 10^6\ M^{-1}{\cdot}s^{-1}$ 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);

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aqueous aerobic $t_{½}$ = 66.7–199 h, based on aerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 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 $t_{½}$ = 1.4 d in adapted activated sludge and k = 0.1 d^{-1} with $t_{½}$ = 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 μM) 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 μM/h for anaerobic batch experiment in serum bottles; k = 1.2 μM/h for dechlorination in anaerobic batch or continuous bioreactor; k = 1.9 μM/h in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999)

Biotransformation: for bacterial transformation k = 1×10^{7} mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982);

degradation rate k = 3.76×10^{-19} mol $cell^{-1}$ h^{-1} (± 47% SD) from pure culture studies, k = 0.02×10^{-14} to 2×10^{-14} mol $cell^{-1} \cdot h^{-1}$ 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);

$t_{½}$ = 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 < 1.5×10^{3} M^{-1} s^{-1} for the reaction with ozone at pH 1.5–3.0 (Hoigné & Bader 1983);

$t_{½}$ = 0.8 h in summer, $t_{½}$ = 3.0 h in winter for distilled water; $t_{½}$ = 0.7 h in summer, $t_{½}$ = 2.0 h in winter for poisoned estuarine water; $t_{½}$ = 0.6 h in summer, $t_{½}$ = 2.0 h in winter for estuarine water, all based on photo-transformation rate under full sunlight and microbes; $t_{½}$ = 8.0 d in summer, $t_{½}$ = 14 d in winter for distilled water; $t_{½}$ = 6 d in summer, $t_{½}$ = 14 d in winter for poisoned estuarine water and $t_{½}$ = 4 d in summer, $t_{½}$ = 17 d in winter for estuarine water, based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986);

$t_{½}$ = 62 h in water at pH 8 and 19 ± 2°C for the reaction with singlet oxygen (Scully & Hoigné 1987);

$t_{½}$ = 2.5–2.6 h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{½}$ = 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 $t_{½}$ = 2.4 min for reaction with Fenton's reagent; $t_{½}$ = 30.4 min at pH 2 and $t_{½}$ = 3.3 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{½}$ = 133–1032 h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: mean half-life of dechlorination: $t_{½}$ = 116 d in July and $t_{½}$ = 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)

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$t_{½}$ = 176–1680 h, based on aerobic soil die-away test data (Baker et al. 1980; Haider et al. 1974; selected, Howard et al. 1991);

$t_{½}$ = 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 & Mattews 1992).

Biota:

TABLE 14.1.2.4.1
Reported aqueous solubilities and vapor pressures of 2,4-dichlorophenol at various temperatures

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}	T/K	S/g·m^{-3}	t/°C	P/Pa
15.3	3896	310.5	6339	294.6	4841	53.0	133.3
25.2	5517	327.1	7244	303.1	6129	80.0	666.6
29.8	6075	338.1	8150	311.5	6683	92.8	1333
35.1	6501	347.2	9056	322.4	7433	107.7	2666
		355.1	9961	336.7	8460	123.4	5333
		363.5	10867	295.2	4939	133.5	7999
		373.7	10867	303.7	6161	146.0	13332
		382.1	11772	312.4	6748	165.2	26664
		393.5	12678	318.1	7139	187.5	53329
		401.5	13583	232.2	7482	210.0	101325
		408.4	14489	291.4	4320		
		423.2	15394	302.0	6047	mp/°C	45.0
				308.8	6504		
				321.0	7335		
				337.7	8525		

*some data from Achard et al. 1996, Jaoui et al. 1999

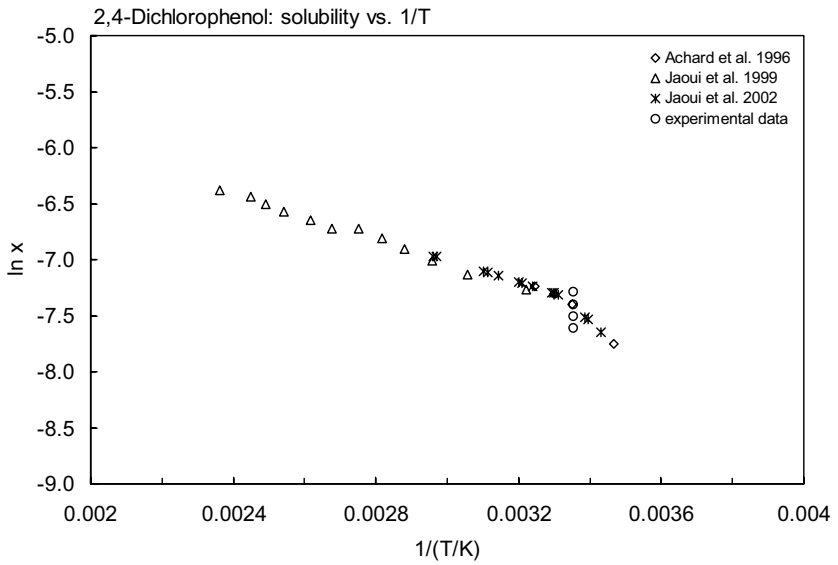

FIGURE 14.1.2.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2,4-dichlorophenol.

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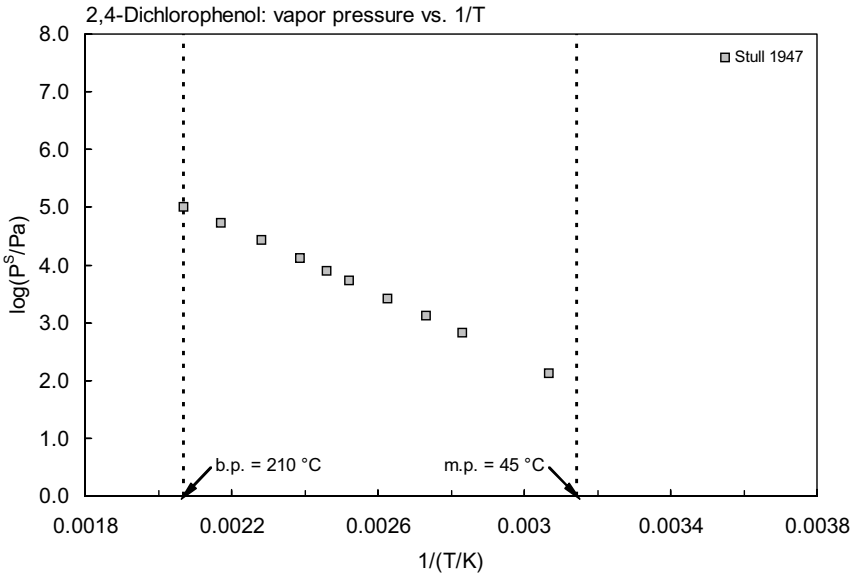

FIGURE 14.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dichlorophenol.

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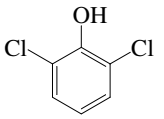
14.1.2.5 2,6-Dichlorophenol



Common Name: 2,6-Dichlorophenol
Synonym: 2,6-DCP
Chemical Name: 2,6-dichlorophenol
CAS Registry No: 87-65-0
Molecular Formula: $C_6H_3Cl_2OH$
Molecular Weight: 163.001
Melting Point (°C):
68.5 (Lide 2003)
Boiling Point (°C):
220 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
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 & Dyrssen 1984; Shigeoka et al. 1988)
6.78 (Ugland et al. 1981; Dean 1985)
6.54 (Nendza & Seydel 1988)
Molar Volume (cm^3/mol):
145.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
22.14 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.374 (mp at 68.5°C)

Water Solubility (g/m^3 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_L/kPa) = 7.32845 – 2436.59/(–35.584 + T/K); temp range 333–493 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/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·m^3/mol at 25°C):
0.7376 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
2.86 (Hansch & Leo 1979)
2.34 (HPLC-RT correlation, Butte et al. 1981)
2.64 (HPLC-k′ correlation, Hammers et al. 1982)

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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 K_{OC}:

Environmental Fate Rate Constants and Half-Lives:
Volatilization:
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 (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $t_{½}$ = 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: $t_{½}$ = 16.2 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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

Stull 1947 summary of literature data	
t/°C	**P/Pa**
59.5	133.3
87.5	666.6
101.0	1333
115.5	2666
131.5	5333
141.8	7999
154.6	13332
175.5	26664
197.7	53329
220.0	101325
mp/°C	-

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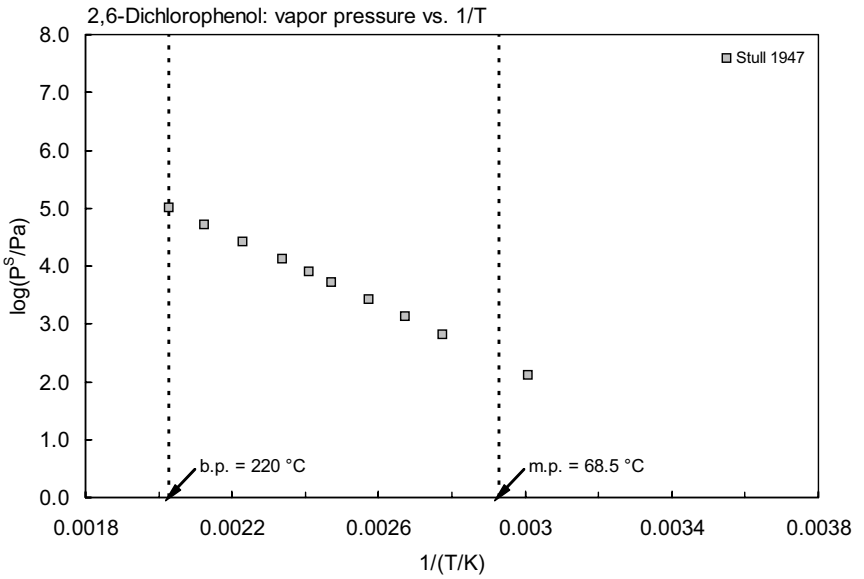

FIGURE 14.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dichlorophenol.

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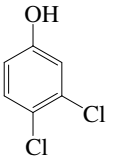
14.1.2.6 3,4-Dichlorophenol



Common Name: 3,4-Dichlorophenol
Synonym: 3,4-DCP
Chemical Name: 3,4-dichlorophenol
CAS Registry No: 95-77-2
Molecular Formula: $C_6H_3Cl_2OH$
Molecular Weight: 163.001
Melting Point (°C):
68.0 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
253 (Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
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)
8.62 (Ugland et al. 1981; Lagas 1988; Renner 1990; Ma et al. 1993)
8.68 (Xie & Dyrssen 1984; Shigeoka et al. 1988; Sangster 1993)
8.63 (Dean 1985)
Molar Volume (cm^3/mol):
145.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.93 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.379 (mp at 68°C)

Water Solubility (g/m^3 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·m^3/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 andrei*: 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)

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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 $^1\chi$, Sabljic et al. 1995)
3.03 (2.93–3.13)	(soil: organic carbon OC ≥ 0.5% and pH ≤ 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 6.84×10^{-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: $t_{½}$ = 115 d in July and $t_{½}$ = 86 d in November with relatively long $t_{½}$ = 66 d reported from site 1, $t_{½}$ = 64 d from site 3 and $t_{½}$ = 132 d from site 5 in January (Hale et al. 1991).
Soil: disappearance $t_{½}$ = 10.1 d from Kooyenburg soil, $t_{½}$ = 11.2 d from Holten soil with earthworms *E. fetida andrei* and $t_{½}$ = 24.7 d from Kooyenburg soil, $t_{½}$ = 49.5 d from Holten soil with earthworms *L. rebellus* (van Gestel & Ma 1988);
$t_{½}$ = 18.3 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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:

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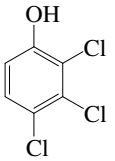
14.1.2.7 2,3,4-Trichlorophenol



Common Name: 2,3,4-Trichlorophenol
Synonym:
Chemical Name: 2,3,4-trichlorophenol
CAS Registry No: 1595-06-0
Molecular Formula: $C_6H_3Cl_3O$, $C_6H_2Cl_3OH$
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/cm^3):
Acid Dissociation Constant, pK_a:
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 (cm^3/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/m^3 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 ($Pa \cdot m^3/mol$):
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)

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Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants and Half-Lives:

Volatilization:
Photolysis: photochemical-transformation $t_{½}$ = 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:

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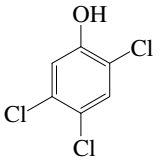
14.1.2.8 2,4,5-Trichlorophenol



Common Name: 2,4,5-Trichlorophenol
Synonym: 245-TCP
Chemical Name: 2,4,5-trichlorophenol
CAS Registry No: 95-95-4
Molecular Formula: $C_6H_2Cl_3OH$
Molecular Weight: 197.446
Melting Point (°C):
69 (Lide 2003)
Boiling Point (°C):
247 (Lide 2003)
Density (g/cm^3 at 20°C):
1.500 (75°C, Verschueren 1983)
Acid Dissociation Constant, pK_a:
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 (cm^3/mol):
166.1 (calculated-Le Bas method at normal boiling point)
165.5 (calculated- χ, Sabljic 1987b)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.59 (exptl., Chickos et al. 1999)
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/m^3 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_L/kPa) = 7.38179 – 2812.25/(–2.091 + T/K); temp range 345–525 K (Antoine eq., Stephenson & Malanowski 1987)
2.93 (calculated, Howard 1991)

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Henry's Law Constant ($Pa \cdot m^3/mol$ 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)
- 3.52; 3.55 (shake flask; HPLC-RT correlation, Wang et al. 1989)
- 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 $\mu g \cdot mL^{-1}$, Call et al. 1980)
- 3.26, 2.82 (total ^{14}C in fathead minnows, observed, calculated, mean exposure level 0.0493 $\mu g \cdot mL^{-1}$, 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 χ, Sabljic 1987a)
- 1.79 (fish, van Gestel & Ma 1988)
- 1.81, 1.53 (earthworms *E. fetida andrei*: 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 χ, 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 $^1\chi$, Sabljic et al. 1995)
- 3.11 (2.81–3.41), 3.35 (3.30–3.40) (soils: organic carbon OC ≥ 0.1% and pH 3.4–6.0, OC ≥ 0.5% and pH ≤ 4.9 undissociated, average, Delle Site 2001)

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

Volatilization: volatilization $t_{½}$ ~ 9.0 d from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{½}$ = 207 d from a model pond (Howard 1991).

Photolysis:

k_P = 1.30 h^{-1} with $t_{½}$ = 0.6 h in summer at mean temp. 25°C and k_P = 0.61 h^{-1} with $t_{½}$ = 1.0 h in winter at mean temp 18°C in distilled water; k_P = 1.2 h^{-1} with $t_{½}$ = 0.6 d in summer and k_P = 0.65 h^{-1} with $t_{½}$ = 1.0 h in winter in poisoned estuarine water; and k_P = 1.4 h^{-1} with $t_{½}$ = 0.5 h in summer and k_P = 0.65 h^{-1} with $t_{½}$ = 1.0 h in winter for estuarine water under full sunlight and microbes (photo-transformation, Hwang et al. 1986)

k_P = 1.30 h^{-1} corresponding to a $t_{½}$ = 0.5 h in summer, k_P = 0.61 h^{-1} corresponding to a $t_{½}$ = 1.0 h in winter in distilled water and k_P = 1.20 h^{-1} corresponding to a $t_{½}$ = 0.6 h in summer, k_P = 0.65 h^{-1} corresponding to a $t_{½}$ = 1.0 h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993)

$t_{½}$ = 0.5–336 h, based on photolysis rate constants for transformation and mineralization under summer and winter, sunlight conditions (Howard et al. 1991)

photolysis $t_{½}$ = 0.6 and 1.0 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, 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:

aqueous photooxidation $t_{½}$ = 66–3480 h in water, based on reported reaction constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

k(aq.) > 10^9 M^{-1} s^{-1} at pH 8, and k < 3 × 10^3 M^{-1} s^{-1} for non-protonated species, k > 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 1.2–1.5 and 20–23°C (Hoigné & Bader 1983b)

k_{OH} = 2.9 × 10^{-12} cm^3 molecule s^{-1} (Bunce et al. 1991)

Hydrolysis: $t_{½}$ > 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 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

aqueous aerobic $t_{½}$ = 552–16560 h, based on unacclimated aerobic river die-away test data (Lee & Ryan 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 3028–43690 h, based on unacclimated anaerobic grab sample data for soil and ground water (Gibson & Suflita 1986; Baker & Mayfield 1980; selected, Howard et al. 1991);

degradation with microbes in darkness negligible (Hwang et al. 1986);

degradation k = 0.00010 d^{-1} with a $t_{½}$ = 16560 h and k = 0.030 d^{-1} with a $t_{½}$ = 552 h for Skidway River water and water-sediment slurry, respectively (Pritchard 1987);

biodegradation $t_{½}$ = 690 d in river water (Howard 1991)

70% reduction in concn (2 μM) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

$t_{½}$(aerobic) = 25 d, $t_{½}$(anaerobic) = 130 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 (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime of 4 d on March 21 at 43°N (Bunce et al. 1991);

$t_{½}$ = 30.1–301 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

$t_{½}$ ~ 7.5 d for reactions with OH radical (estimated, Howard 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: 840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

Rate constant k < 3 × 10^3 M^{-1} s^{-1} for the reaction with O_3 at pH 1.2–1.5 (Hoigné & Bader 1983);

$t_{½}$ = 0.5 h (summer), $t_{½}$ = 1.0 h (winter) in distilled water and $t_{½}$ = 0.5 h (summer), $t_{½}$ = 1.0 h (winter) in surface estuarine water based on photo-transformation rate under full sunlight and microbes (Hwang et al. 1986);

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$t_{½}$ = 7 d (summer), $t_{½}$ = 14 d (winter) in distilled water and $t_{½}$ = 3 d (summer), $t_{½}$ = 8 d (winter) in estuarine water based on photo-mineralization rater under full sunlight and microbes (Hwang et al. 1986);
$t_{½}$ = 0.6 h (summer), $t_{½}$ = 1.0 h (winter) in poisoned estuarine water based on photo-transformation rate and $t_{½}$ = 6 d (summer), $t_{½}$ = 14 d (winter) in poisoned estuarine water based on photomineralization rate (Hwang et al. 1986);
$t_{½}$ = 16560 h at 21°C in Skidway River water (Pritchard 1987);
photodegradation $t_{½}$ = 0.5 h (summer), $t_{½}$ = 1.0 h (winter) in distilled water and $t_{½}$ = 0.6 h (summer), $t_{½}$ = 1.0 h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993);
$t_{½}$ = 0.5–336 h, based on aqueous photolysis half-life (Howard et al. 1991); rapidly photolyze with a $t_{½}$ = 0.6–1.0 h at water surfaces, $t_{½}$ = 690 d in water column (Howard 1991)
t_2(aerobic) = 25 d, t_2(anaerobic) = 130 d in natural waters (Capel & Larson 1995)

Ground water: $t_{½}$ =1104–43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{½}$ = 23 d from calculated degradation rate constant k = 0.0030 d^{-1} for radiolabeled 2,4,5-TCP in Skidway River water-sediment slurry (Lee & Ryan 1979; quoted, Pritchard 1987);
biodegradation $t_{½}$ = 23 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 $t_{½}$ = 3.4 d from Kooyenburg soil and $t_{½}$ = 6.6 d from Holten soil with earthworms *E. fetida andrei* and $t_{½}$ = 39.6 d from Kooyenburg soil, $t_{½}$ = 13.9 d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988);
$t_{½}$ = 33 d in sandy loam (Kjeldsen et al. 1990)
$t_{½}$ = 552–16560 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); under aerobic conditions biodegradation $t_{½}$ = 15 d in a soil suspension (Howard 1991);
$t_{½}$ = 22.3 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 14.6 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota: depuration $t_{½}$(obs.) = 12 h, $t_{½}$(calc) = 9.2 h for mean exposure level of 0.0048 μg·mL^{-1} and $t_{½}$(obs) = 12 h, $t_{½}$(calc) = 6.6 h for mean exposure level of 0.0493 μg·mL^{-1} (fathead minnow, Call et al. 1980).

TABLE 14.1.2.8.1
Reported vapor pressures of 2,4,5-trichlorophenol at various temperatures

Stull 1947	
summary of literature data	
t/°C	**P/Pa**
72.0	133.3
102.1	666.6
117.3	1333
134.0	2666
151.5	5333
162.5	7999
178.0	13332
201.5	26664
226.5	53329
251.8	101325
mp/°C	62

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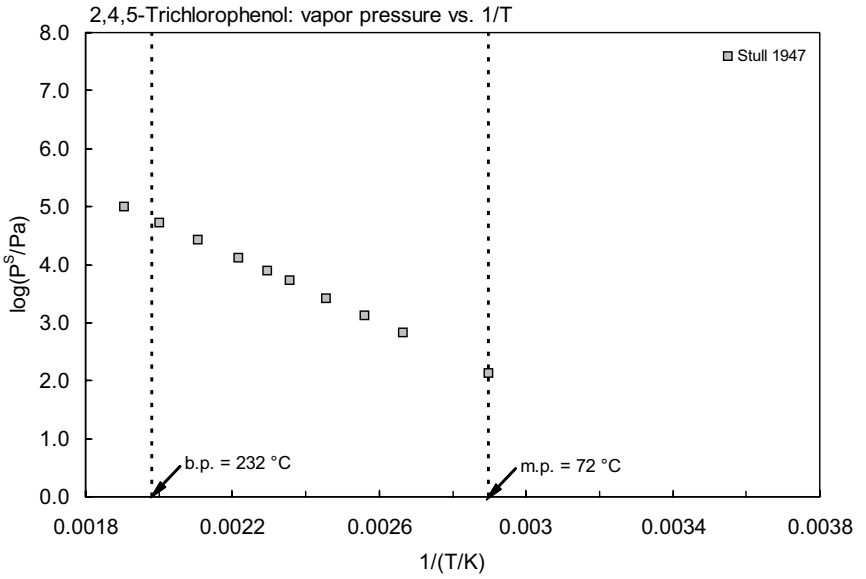

FIGURE 14.1.2.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,5-trichlorophenol.

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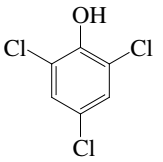
14.1.2.9 2,4,6-Trichlorophenol



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: $C_6H_2Cl_3OH$
Molecular Weight: 197.446
Melting Point (°C):
69 (Lide 2003)
Boiling Point (°C):
246.0 (Stull 1947; Weast 1982–83; Lide 2003)
Density (g/cm^3):
1.675 (Schmidt-Bleek et al. 1982)
1.491 (75°C, Weast 1982–83)
Acid Dissociation Constant, pK_a:
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 (cm^3/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/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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)
$312 \times (1 + 10^{pH-6.06})$ (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 294.9–317.2 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 exptl. 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 exptl. data, Jaoui et al. 2002)

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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 P_L, Bidleman & Renberg 1985)
4.28 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/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·m^3/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)
$0.523/(1 + 10^{pH + 6.06})$ (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 K_{OW}:

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 & Viluksela 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, Körte et al. 1978)
1.60, 1.71, 2.49 (activated sludge, algae, golden orfe, Freitag et al. 1982)
1.71; 1.81 (algae: exptl; calculated, Geyer et al. 1981)
1.54–1.78, 1.60 (mussel *mytilus edulis*, Geyer et al. 1982)
2.92 (microorganisms-water, calculated-K_{OW}, 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)

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1.71, 2.13 (algae: exptl., calculated-K_{OW}, 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)
2.75; 2.84 (Atlantic salmon fry: humic water; lake water, Carlberg et al. 1986)
1.30 (Isnard & Lambert 1988)
1.94; 2.83 (flagfish: whole fish; fish lipid, Smith et al. 1990)
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_{OC}:

2.34 (sediment, Virtanen & Hattula 1982)
3.30 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.52 (soil, Seip et al. 1986)
3.41–3.84 (soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.33–3.57 (soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.52–2.75 (soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987a,b)
3.30–3.73 (soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987a,b)
2.48–2.87 (soil, calculated-K_{OW}, 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)
3.34, 2.79, 2.23 (average values, soil at pH 6, 7, and 7.7, Yoshida et al. 1987)
2.79, 3.34, 2.04 (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)
2.50 (soil, calculated-MCI χ, Bahnick & Doucette 1988)
2.92–3.12; 3.03 (lit. range, mean value, Robinson & Novak 1994)
2.82–3.02 (log K_{OM}, organic matter, Robinson & Novak 1994)
2.81, 3.03 (log K_{HA}, humic acid, Robinson & Novak 1994)
2.25 (calculated-K_{OW}, Kollig 1993)
3.02 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.59; 3.08 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
2.52 (1.97–3.01), 2.88 (2.33–3.39) (soils: organic carbon OC ≥ 0.1% and pH > 4.2, OC ≥ 0.1% and pH ≤ 4.2 undissociated, average, Delle Site 2001)

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

Volatilization: volatilization and sorption $t_{½}$ ~ 192 h from natural pond (Schauerte et al. 1982);
volatilization rate constant from water $k = 3.90 \times 10^{-3}/(1 + 10^{pH-6.06})/L_w$ h^{-1}, L_w, depth of water phase (Yoshida et al. 1987).

Photolysis: aqueous photolysis $t_{½}$ = 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);
photo-degradation rate constants $k_p = (0.156 + 9.16 \times 10^{pH-5.86})/(1 + 10^{pH-5.86})^{-1}$ in water, for summer, fine day, and $k_p = (0.042 + 1.40 \times 10^{pH-6.09})/((1 + 10^{pH-6.09})$ h^{-1} in water, for winter, fine day; k = 0.72 d^{-1} for river, k = 2.2 d^{-1} for oligotrophic lake and k = 0.776 d^{-1} for eutrophic lake (Yoshida et al. 1987);
photochemical-transformation $t_{½}$ = 1.2 h in Xenotest 1200 (Svenson & Björndal 1988);
photolysis $t_{½}$ = 24 h (Paasivirta 1992);
photo-degradation rate constant $k = 26 \times 10^3$ min^{-1} with $t_{½}$ = 25.2 min for direct UV radiation aqueous solutions (Benitez et al. 2000).

Oxidation: aqueous oxidation rate constant $k < 7 \times 10^4$ M^{-1} h^{-1} for singlet oxygen and $k = 1 \times 10^6$ M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);
apparent reaction rate constant $k > 10^8$ $M^{-1} \cdot s^{-1}$ at pH 8, and rate constants $k < 10^4$ M^{-1} s^{-1} for non-protonated species, $k > 10^8$ 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);

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photooxidation $t_{½}$ = 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 $t_{½}$ = 20.3–2027 h, based on measured rate data for reaction with singlet oxygen in aqueous solution (Scully & Hoigne 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, $k = 2.6 \times 10^7$ $M^{-1} \cdot s^{-1}$ 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 ± 2)°C (Scully & Hoigné 1987);
rate 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 ± 1°C (Tratnyek & Hoigné 1991);
photo-oxidation rate constant $k = 98 \times 10^3$ min^{-1} with $t_{½}$ = 5.1 min for reaction with Fenton's reagent; and $k = 44 \times 10^3$ min^{-1} with $t_{½}$ = 20.6 min at pH 2 and $k = 314 \times 10^3$ min^{-1} with $t_{½}$ = 3.1 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: $t_{½} > 8 \times 10^6$ yr, based on hydrolysis rate constant of zero at pH 7 (Kollig et al. 1987; quoted, Howard et al. 1991).

Biodegradation: $t_{½}$ = 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, Verschueren 1983);
$t_{½}$ = 216–432 h and 624–1560 h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);
aqueous aerobic $t_{½}$ = 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 $t_{½}$ = 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 $cell^{-1} \cdot h^{-1}$ at 20°C and pH 7;
biodegradation rate constants $k = 8.4 \times 10^{-5}$ 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_2 = 4.78 d^{-1}, 2.54 d^{-1} (fish: bioconcentration based; toxicity based, Smith et al. 1990)

Half-Lives in the Environment:

Air: $t_{½}$ = 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 > 5d (Kelly et al. 1994).

Surface water: $t_{½}$ = 216–432 h and 624–1560 h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);
$t_{½}$ = 1.2 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
$t_{½}$ = 2–96 h, based on aqueous photolysis half-life (Sugiura et al. 1984; quoted, Howard et al. 1991);
$t_{½}$ = 62 h for the reaction with singlet oxygen at pH 8 and (19 ± 2)°C in water (Scully & Hoigné 1987)
photolysis $t_{½}$ = 24 h (Paasivirta 1992);
photo-oxidation $t_{½}$ = 5.1 min for reaction with Fenton's reagent; $t_{½}$ = 20.6 min at pH 2 and $t_{½}$ = 3.1 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

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Ground water: $t_{½}$ = 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)

$t_{½}$ = 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);

$t_{½}$ = 6.3 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 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);

$t_{½}$ = 6720 h (Paasivirta 1992).

Biota: $t_{½}$ = 0.15 d of clearance from whole flagfish; $t_{½}$ = 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

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}	T/K	S/g·m^{-3}	t/°C	P/Pa
19.5	410	314.2	1144	294.9	493.6	76.5	133.3
20.1	427	334.3	1376	304.6	947.8	105.9	666.6
24.9	692	335.3	1377	308.6	933.1	120.2	1333
30.0	928	337.6	1733	314.6	1362	135.8	2666
		342.3	2116	320.9	1323	152.2	5333
		345.3	2377	294.9	493.6	163.5	7999
		352.2	2832	297.7	631.8	177.8	13332
		369.9	3391	302.4	908.3	199.0	26664
		383.8	5419	307.5	1007	222.5	53329
		408.1	7086	313.7	1145	246.0	101325
		420.6	7777	292.8	414.6		
				302.2	888.5	mp/°C	68.5
				308.0	1007		
				317.2	1224		
				some data from Achard et al. 1996, Jaoui et al. 1999			

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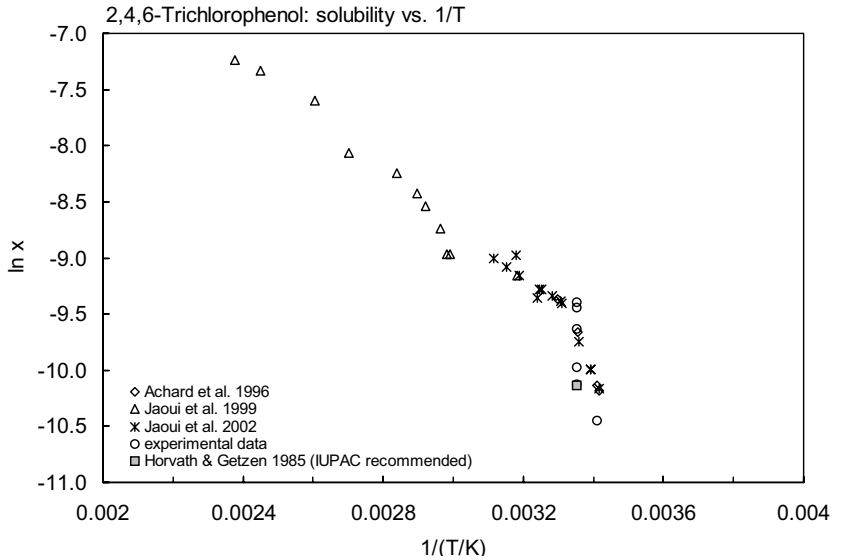

FIGURE 14.1.2.9.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2,4,6-trichlorophenol.

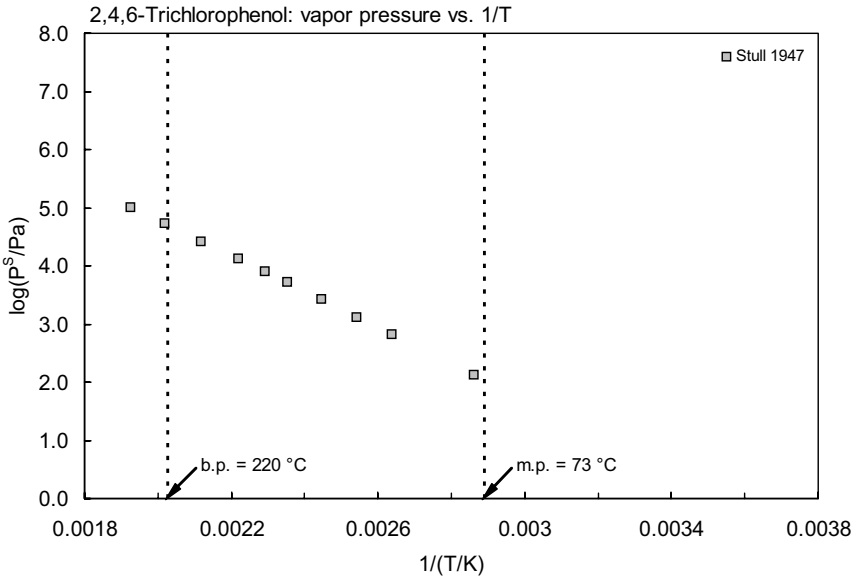

FIGURE 14.1.2.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorophenol.

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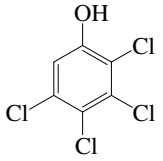
14.1.2.10 2,3,4,5-Tetrachlorophenol



Common Name: 2,3,4,5-Tetrachlorophenol
Synonym:
Chemical Name: 2,3,4,5-tetrachlorophenol
CAS Registry No: 4901-51-3
Molecular Formula: C_6HCl_4OH
Molecular Weight: 231.891
Melting Point (°C):
116.5 (Lide 2003)
Boiling Point (°C):
sublimation (Weast 1982–83; Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
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 (cm^3/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: 0.127 (mp at 116.5°C)

Water Solubility (g/m^3 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 m^3/mol):
0.140 (calculated-P/C, Shiu et al. 1994)

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

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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, 2.73, 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, $t_{½}$:

Volatilization:
Photolysis: photochemical transformation $t_{½}$ = 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 $k = 7.14 \times 10^{-22}$ (± 41% SD) mol·cell^{-1}·h^{-1} from pure culture studies and $k = 5 \times 10^{-16}$ 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: $t_{½}$ = 0.88 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).
Ground water:
Sediment:
Soil: disappearance $t_{½}$ = 43.4 d from Kooyenburg soil, $t_{½}$ = 29.1 d from Holten soil with earthworm *E. fetida andrei* and $t_{½}$ = 26.8 d from Kooyenburg soil, $t_{½}$ = 42.5 d from Holten soil with earthworm *L. rebellus* (van Gestel & Ma 1988).
Biota:

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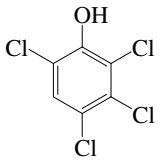
14.1.2.11 2,3,4,6-Tetrachlorophenol



Common Name: 2,3,4,6-Tetrachlorophenol
Synonym:
Chemical Name: 2,3,4,6-tetrachlorophenol
CAS Registry No: 58-90-3
Molecular Formula: C_6HCl_4OH
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/cm^3):
1.60 (at 60°C, Verschueren 1983)
Acid Dissociation Constant, pK_a:
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 (Ugland 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 (cm^3/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: 0.362 (mp at 70°C)

Water Solubility (g/m^3 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_L/kPa) = 7.96172 – 3227.92/(–6.121 + T/K); temp range 373–548 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):
0.3548 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
4.10 (Hansch & Leo 1979)
4.27 (RP-HPLC-k′ correlation, Miyake & Terada 1982)
4.45 (shake flask-GC, Saarikoski & Viluksela 1982)

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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)
4.42 (OECD 1981 guidelines, Leuenberger et al. 1985)
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_{OC}:

4.21 (soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.77 (soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.94 (soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987a,b)
4.11 (soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987a,b)
3.20 (soil, calculated-K_{OW}, 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 $^1\chi$, 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, $t_{½}$:

Volatilization:
Photolysis: aqueous photolysis $t_{½}$ ~ 1–336 h, based on aqueous data for 24,5- 2,4,6-trichlorophenols and pentachlorophenol (Howard et al. 1991);
photo-degradation rate constant $k = 21 \times 10^3$ min^{-1} with $t_{½}$ = 30.6 min for direct UV radiation aqueous solutions (Benitez et al. 2000).
Photooxidation: atmospheric $t_{½}$ = 364.4–3644 h, based on estimated rate constant for reaction with OH radical and aqueous $t_{½}$ = 66.0–3480 h, based on reaction rate constants with OH and $RO_2\cdot$ radicals with phenol class (Howard et al. 1991);
photo-oxidation rate constant $k = 9 \times 10^3$ min^{-1} with $t_{½}$ = 49.5 min for reaction with Fenton's reagent; and $k = 94 \times 10^3$ min^{-1} with $t_{½}$ = 10.6 min at pH 2 and $k = 415 \times 10^3$ min^{-1} with $t_{½}$ = 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: $t_{½}$ > 72 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983);
aqueous aerobic $t_{½}$ = 672–4032 h, based on acclimated aerobic screening test data and aqueous anaerobic $t_{½}$ = 2688–16128 h, based on unacclimated aerobic biodegradation half-lives (Howard et al. 1991).
Biotransformation:
Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

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Half-Lives in the Environment:

Air: $t_{½}$ = 364.4–3644 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{½}$ = 0.88 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
$t_{½}$ = 1–336 h, based on estimated aqueous photolysis data for trichlorophenols and PCP (Howard et al. 1991);
photo-oxidation $t_{½}$ = 49.5 min for reaction with Fenton's reagent; $t_{½}$ = 10.6 min at pH 2, and $t_{½}$ = 1.9 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{½}$ = 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)
$t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

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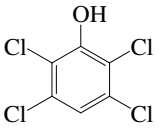
14.1.2.12 2,3,5,6-Tetrachlorophenol



Common Name: 2,3,5,6-Tetrachlorophenol
Synonym:
Chemical Name: 2,3,5,6-tetrachlorophenol
CAS Registry No: 935-95-5
Molecular Formula: $C_6H_2Cl_4O$, C_6HCl_4OH
Molecular Weight: 231.891
Melting Point (°C):
115 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
5.30 (Sillen & Martell 1971)
5.03 (Konemann 1981; Ugland et al. 1981)
5.40 (Sangster 1993)
Molar Volume (cm^3/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/m^3 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 m^3/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, $t_{½}$, 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 (k_1 and k_2):

Half-Lives in the Environment:

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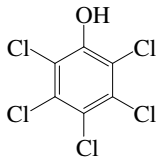
14.1.2.13 Pentachlorophenol



Common Name: Pentachlorophenol
Synonym: chlorophen, PCP, penchlorol
Chemical Name: pentachlorophenol
CAS Registry No: 87-86-5
Molecular Formula: C_6Cl_5OH
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/cm^3):
- 1.987 (Firestone 1977)
- 1.978 (22°C, Weast 1982–83)

Acid Dissociation Constant, pK_a:
- 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 & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)
- 4.60 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):
- 207.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 17.5 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0350 (mp at 174°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- 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)
- 21.4* (25.1°C, shake flask-conductimetry, measured range 25.1–46.8°C, Achard et al. 1996)

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13.0 (shake flask-HPLC/UV, pH 4.55, Huang et al. 2000)
102* (60.05°C, shake flask-optical method, measured range 333.2–422.3 K, Jaoui et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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) = [–0.2185 × 16742.6/(T/K)] + 9.150200; temp range 192.2–309.3°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), temp range 200–253°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), 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·m^3/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_{OW}:
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, Veith 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 & Viluksela 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)
3.69, 3.81 (shake flask, OECD 1981 Guidelines, Geyer et al. 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)
5.24 (OECD 1981 guidelines, Leuenberger et al. 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)

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5.00 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
5.18 (recommended, LOGKOW databank, Sangster 1993)
5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
5.02 (shake flask-GC/ECD, Kishino & Kobayashi 1994)
5.12 (recommended, pH 1.4, Hansch et al. 1995)
4.74, 4.60, 4.27, 3.69, 3.59 (pH 2.1–3.1, 5.0, 6.1, 7.2, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase), measured range pH 2.1–13.3, Nowosielski & Fein 1998)

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: exptl., 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 (*alga Chlorella fusca* in culture flasks, Geyer et al. 1984; quoted, Brockway et al. 1984)
3.10, 2.72 (algae: exptl, 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*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
1.35 (whole *lumbricus terrestris*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
2.89 (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_B/C_W, Mäenpää et al. 2004)

Sorption Partition Coefficient, log K_{OC}:

2.95 (soil, calculated-K_{OW}, Kenaga & Goring 1980)
4.72 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

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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 χ, Sabljic 1987a,b)
2.95 (soil, calculated-MCI χ, 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, 5.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
5.58, 5.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)
4.51, 4.54 (neutral form, silt-clay slurries, Jafvert & Weber 1991)
3.06 (calculated-K_{OW}, Kollig 1993)
3.73 (soil, calculated-MCI $^1\chi$, 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 ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 2.0- > 10, average, Delle Site 2001)
3.38, 3.51, 2.92 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 3.4–6.9, average, Delle Site 2001)
4.48, 4.54, 4.38 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH ≤ 3 undissociated, average, Delle Site 2001)
2.82, 2.89, 2.63 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH –7.1 dissociated, average, Delle Site 2001)

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

Volatilization/evaporation: $t_{½}$ = 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 7×10^{-6} m^2/s and in water 7×10^{-10} m^2/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);
k(calc) = 5×10^{-4} d^{-1} to 1×10^{-7} d^{-1} for total PCP (Crossland & Wolff 1985).

Photolysis: photolysis: $t_{½}$(calc) = 4.75 h from observed rate k = 3.4×10^{-4} s^{-1} for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm^2 between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
photolysis $t_{½}$ = 1.5 d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);
photolytic $t_{½}$ = 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 $t_{½}$ = 1.5 to 3.0 d (Crossland & Wolff 1985);
photo-transformation rate constants k = 0.6 h^{-1} with $t_{½}$ = 1 h for distilled water in summer (mean temperature 25°C) and k = 0.37 h^{-1} with $t_{½}$ = 2 h in winter (mean temperature 11°C); k = 0.37 h^{-1} with $t_{½}$ = 2 h for

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both poisoned estuarine water and estuarine water in summer and k = 0.27 h^{-1} with $t_{½}$ = 3 h in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
photo-mineralization rate constants k = 0.11 h^{-1} with $t_{½}$ = 6 d for distilled water in summer (mean temperature 25°C) and k = 0.049 h^{-1} with $t_{½}$ = 14 d in winter (mean temperature 11°C); k = 0.12 h^{-1} with $t_{½}$ = of 6 d for poisoned estuarine water in summer and $t_{½}$ = 0.07 h^{-1} with $t_{½}$ = 10 d in winter; k = 0.25 h^{-1} with $t_{½}$ = 10 d for estuarine water in summer and k = 0.10 h^{-1} with $t_{½}$ = 7 d for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
photochemical transformation $t_{½}$ = 0.75 h in Xenotest 1200 (Svenson & Björndal 1988);
aqueous $t_{½}$ = 1–110 h (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991)
$t_{½}$ = 7.43 d, assuming a linear rate of photolysis during 96-h period,(Smith et al. 1987)
photodegradation k = 0.60 h^{-1} corresponding to a $t_{½}$ = 1.0 h (summer), k = 0.37 h^{-1} corresponding to a $t_{½}$ = 2 h (winter) in distilled water; and $t_{½}$ = 0.37 h^{-1} corresponding to a $t_{½}$ = 2 h (summer), 0.27 h^{-1} corresponding to a $t_{½}$ = 3.0 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 < 7×10^3 M^{-1} h^{-1} for singlet oxygen and k = 1×10^5 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);
k >> 3.0×10^5 M^{-1} s^{-1} with 3 mM AcOH as scavenger for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983b);
photooxidation $t_{½}$ = 66–3480 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; Güesten et al. 1981; quoted, Howard et al. 1991);
photooxidation $t_{½}$ = 139.2–1392 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
rate constant k = 4.7×10^{-13} cm^3 molecule s^{-1} for reaction with OH radical in air (Bunce et al. 1991)
rate constant k = $(0.2 \pm 5.5) \times 10^6$ M^{-1} s^{-1} for the reaction with singlet oxygen in aqueous phosphate buffer at 27 ± 1°C (Tratnyek & Hoigné 1991);
atmospheric $t_{½}$ < 24 h at noon in mid-summer to $t_{½}$ = 216 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 = 7.4×10^{-4} h^{-1} in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983);
$t_{½}$ = 1800–2160 h and 480-∞ h to obtain 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);
k = 0.10 d^{-1} with a $t_{½}$ = 7 d in unadapted Nutrient Broth and k = 1.0 d^{-1} with a $t_{½}$ = 0.7 d in adapted Nutrient Broth under aerobic conditions (Mills et al. 1982);
aqueous aerobic $t_{½}$ = 552–4272 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 $t_{½}$ = 1008–36480 h, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);
aerobic degradation rate constant k = 0.0017 L $\mu g^{-1} \cdot d^{-1}$ (Moos et al. 1983);
microbial degradation negligible in darkness (Hwang et al. 1986);
100% reduction in concn (2 µM) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)
degradation rate constant k = 0.12 ± 0.01 h^{-1} in the absence of light (Minero et al. 1993).
$t_{½}$(aerobic) = 23 d, $t_{½}$(anaerobic) = 42 d in natural waters (Capel & Larson 1995)

Biotransformation: first order fish metabolism k = 1.5×10^{-5} h^{-1} (Sanborn et al. 1975, quoted, Addision et al. 1983);
bacterial transformation k = 3×10^9 mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982);
degradation rate k = 3×10^{-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:
k_1 = 18.3 h^{-1}, 19 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 d^{-1}, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)
k_2 = 1.03 d^{-1}, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

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k_2 = 1.03 d^{-1}, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)
k_2 = 0.00195 ± 0.00063 h^{-1} (*m. relicta*, Landrum & Dupuis 1990)
k_2 = 0.00330 ± 0.00140 h^{-1} (*p. hoyi*, Landrum & Dupuis 1990)
k_1 = 662.4 d^{-1}, k_2 = 0.502 d^{-1} (algae *Chlorella fusca*, Wang et al. 1996)
k_1 = 0.733 d^{-1}, k_2 = 0.020 d^{-1} (eggshell of dissected parts of lake salmon, Mäenpää et al. 2004)
k_1 = 0.680 d^{-1}, k_2 = 0.000 d^{-1} (yolk sac of dissected parts of lake salmon, Mäenpää et al. 2004)
k_1 = 2.828 d^{-1}, k_2 = 0.015 d^{-1} (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);
$t_{½}$ = 139.2–1392 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radicals in air; photolysis $t_{½}$ = 6.5 h in noonday summer sunshine (Howard 1991);
atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: calculated photolysis $t_{½}$ = 4.75 h from a determined rate k = 3.4×10^{-4} s^{-1} for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm^2 between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
photolysis $t_{½}$ = 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);
photolytic $t_{½}$ = 10–15 d (Brockway et al. 1984);
rate constant k >> 3.0×10^5 M^{-1} s^{-1} for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);
estimated direct photolysis midday $t_{½}$ = 20 min from experimentally determined rate constant k = 2.1 h^{-1} (quoted unpublished result, Zepp et al. 1984);
$t_{½}$ = 1.5 to 3.0 d for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);
$t_{½}$ = 1 h (summer), $t_{½}$ = 2 h (winter) for distilled water; $t_{½}$ = 2 h (summer), $t_{½}$ = 3 h (winter) for estuarine water; $t_{½}$ = 2 h (summer), $t_{½}$ = 3 h (winter) for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986); $t_{½}$ = 6 d (summer), $t_{½}$ = 14 d (winter) for distilled water; $t_{½}$ = 3 d (summer), $t_{½}$ = 7 d (winter) for estuarine water; $t_{½}$ = 6 d (summer), $t_{½}$ = 10 d (winter) for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);
$t_{½}$ = 0.75 h and 0.96 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
$t_{½}$ = 1–110 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 $t_{½}$ = 1.0 h (summer), $t_{½}$ = 2.0 h (winter) in distilled water and $t_{½}$ = 2.0 h (summer), $t_{½}$ = 3.0 h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).
$t_{½}$(aerobic) = 23 d, $t_{½}$(anaerobic) = 42 d in natural waters (Capel & Larson 1995)

Ground water: $t_{½}$ = 1104–36480 h, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et at. 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 = 7.4×10^{-4} h^{-1} 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 $t_{½}$ = 23.2 d from Kooyenburg soil, $t_{½}$ = 47.9 d from Holten soil with earthworm *e. fetida andrei* and $t_{½}$ = 27.4 d from Kooyenburg soil, $t_{½}$ = 31.8 d from Holten soil with earthworm *l. rubellus* (van Gestel & Ma 1988);
$t_{½}$ = 552–4272 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{½}$ = 2.0 d in an acidic clay soil with < 1.0% organic matter and $t_{½}$ = 6.7 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota: biological $t_{½}$ = 30 d in guppy *lebistes reticulatus*(Landner et al. 1977);
elimination $t_{½}$ = 23, 9.3, 6.9, and 6.2 h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);
estimated $t_{½}$ = 7.0 d in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);
clearance from flagfish: $t_{½}$ = 0.68 d from whole fish and $t_{½}$ = 0.68 d from fish lipid (Smith et al. 1990).

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TABLE 14.1.2.13.1
Reported aqueous solubilities of pentachlorophenol at various temperatures

Carswell & Nason 1938		Achard et al. 1996		Jaoui et al. 1999	
shake flask		shake flask-conductivity		static visual method	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}
0	5	25.1	21.4	333.2	102
27	18	34.5	57.8	342.7	118.4
50	35	46.8	86.2	353.2	140.6
62	58			361.2	156.8
70	85			372.0	173.1
				386.0	195.3
				402.0	211.6
				407.0	232.3
				422.3	253.0

Note: PCP data in Table I incorrect, correction made Figure 3 in ref based on Figure 3 in ref.

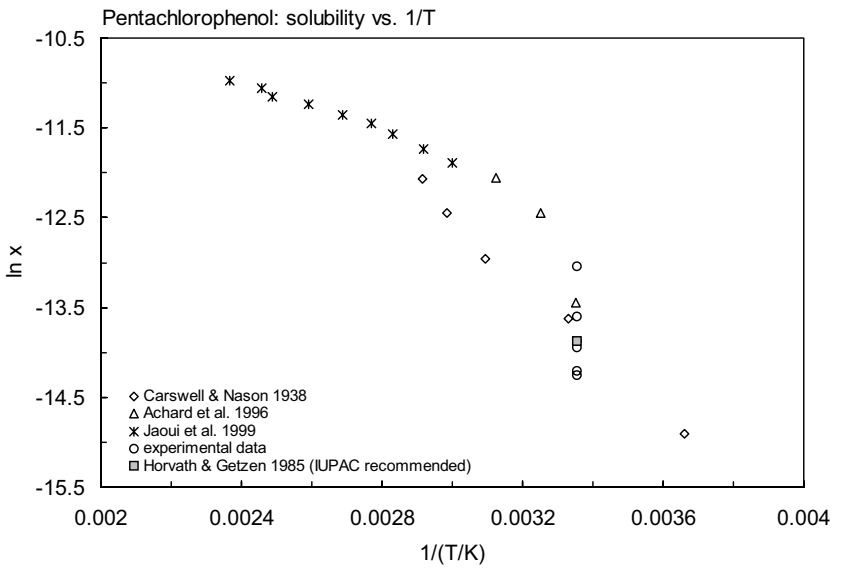

FIGURE 14.1.2.13.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for pentachlorophenol.

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TABLE 14.1.2.13.2
Reported vapor pressures of pentachlorophenol 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)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Carswell & Nason 1938		Stull 1947		McDonald et al. 1959		Rordorf 1989	
static method		summary of literature data		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	0.00227*	192.2	2666	46.0	0.108	25	0.0070
20	0.0227*	211.2	5333	60.0	0.1853	50	0.110
50	0.4133*	223.4	7999	70.0	0.2573	75	1.20
75	3.200*	239.6	13332	71.8	0.3960	100	9.50
100	18.67	261.8	26664	80.0	0.9746	125	57.0
120	63.99	285.0	53329	93.6	3.3597		
140	200.0	309.3	101325	106.5	8.5460		for solid
160	573.3			119.5	23.60	eq. 1	P_S/Pa
180	1453	mp/°C	188.5	200.6	4133	A	13.413
200	3413			215.51	6759	B	4640.9
220	7493			233.87	12279		
240	14705*						for liquid
260	30358*			eq. 2	P/mmHg	eq. 1	P_L/Pa
280	56622*			A	9.073	A	11.47085
300	101112*			B	3606.0	B	3750.68
300.6	101325			C	273.15		
measured range 100–220°C				mp/°C	189.65		
*extrapolated from graph				.			

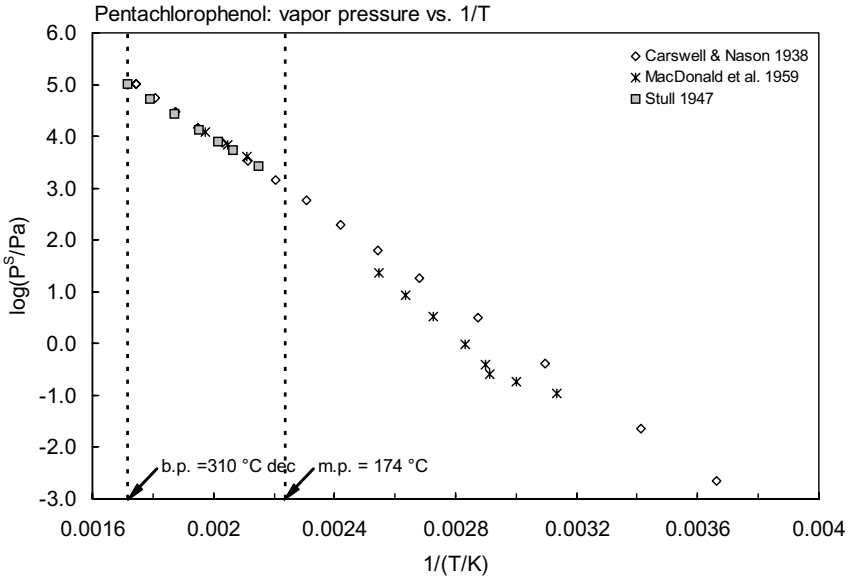

FIGURE 14.1.2.13.2 Logarithm of vapor pressure versus reciprocal temperature for pentachlorophenol.

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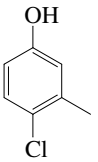
14.1.2.14 4-Chloro-*m*-cresol



Common Name: 4-Chloro-*m*-cresol
Synonym: *p*-chloro-*m*-cresol, 2-chloro-5-hydroxytoluene, 4-chloro-3-methylphenol
Chemical Name: 4-chloro-*m*-cresol, 4-chloro-3-methylphenol
CAS Registry No: 59-50-7
Molecular Formula: C_7H_7ClO, $CH_3(Cl)C_6H_3OH$
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/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/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/m^3 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 m^3/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, k, and Half-Lives, $t_{½}$:
Oxidation: rate constants $k < 7 \times 10^5$ M^{-1} h^{-1} for singlet oxygen and $k = 1 \times 10^7$ M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982).
Biotransformation: bacterial transformation $k = 3 \times 10^{-9}$ mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982).

Half-Lives in the Environment:

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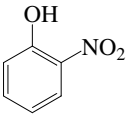
14.1.3 NITROPHENOLS

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: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$
Molecular Weight: 139.109
Melting Point (°C):
44.8 (Lide 2003)
Boiling Point (°C):
216.0 (Weast 1982-83; Lide 2003)
Density (g/cm^3 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, pK_a:
7.21 (Pearce & Simkins 1968)
7.23 (Serjeant & Dempsey 1979)
8.28 (Mabey et al. 1982)
7.22 (Dean 1985)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.57 (Tsonopoulos & Prausnitz 1971)
17.44 (Beneš & Dohnal 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55.23 (Tsonopoulos & Prausnitz 1971)
48.95, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.630 (mp at 44.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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)

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24.43 (extrapolated-Cox eq., Chao et al. 1983)
log (P/mmHg) = [1– 487.905/(T/K)] × 10^{0.885400 – 6.30106 × 10^{-4}·(T/K) + 6.42867 × 10^{-7}·$(T/K)^2$}; 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_S/kPa) = 7.8446 – 2864.6/(T/K), temp range 273–292 K (solid, Antoine eq-I., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.04963 – 1571.7/(–101.17 + T/K), 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 ΔS_{fus} and mp, Schwarzenbach et al. 1988)
log (P/atm) = 5.735 – 2776/(T/K) (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

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):
0.766 (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=/(M atm^{-1})] = 6290/(T/K) – 16.6; 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/(M atm^{-1})] = 6270/(T/K) – 16.6; temp range 284–302 K, Harrison et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
1.79 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971)
2.00 (shake flask, Umeyama et al. 1971)
1.25, 1.18 (calculated-fragment const., calculated-π 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_{OW}, Mabey et al. 1982)
1.15 (calculated-K_{OW}, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
1.43 (sediment-water, calculated-K_{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)
2.424, 1.507, 1.852, 1.763, 2.336 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.043, 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)

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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 and HPLC-k′ correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: volatilization $t_{½}$ = 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 NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

rate constant $k < 2 \times 10^5$ $M^{-1}{\cdot}h^{-1}$ for singlet oxygen, and $k = 2 \times 10^6$ $M^{-1}{\cdot}h^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k_{OH} = 0.922 \times 10^{-12}$ $cm^3{\cdot}molecule^{-1}{\cdot}s^{-1}$ at 296 K (Becker et al. 1984; quoted, Carlier et al. 1986);

k_{OH}(exptl) = 0.92×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 3.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1985)

k_{OH}(exptl) = 0.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 4.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1987)

$k_{OH} = 0.90 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 294 K (Atkinson 1989)

photooxidation $t_{½}$ = 7–71 h, based on measured rate data for the vapor phase reaction with OH radical in air (Howard et al. 1991)

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

$k_{OH} = (2.34 \pm 0.33) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at (24.6 ± 0.4)°C (Edney et al. 1986)

$k_{OH} = 2.34 \times 10^{-12}$ $cm^3{\cdot}molecule^{-1}$ s^{-1} at 298 K, $k_{NO3} = 9.7 \times 10^{-17}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (Atkinson 1990)

$k_{NO3} < 0.02 \times 10^{-12}$ $cm^3{\cdot}molecule^{-1}$ s^{-1} at 296 K and $k_{OH} = 0.90 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1991)

aqueous photooxidation $t_{½}$ = 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 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);

average rate of biodegradation 14.0 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);

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 $t_{½}$ = 168–672 h, based on unacclimated aerobic screening test data (Sasaki 1978; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{½}$ = 168–672 h, based on anaerobic soil grab sample data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991).

Biotransformation: estimated bacterial transformation rate constant of 2×10^{-9} $mL{\cdot}cell^{-1}{\cdot}h^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{½}$ = 14 h for the gas phase reaction with hydroxyl radical (GEMS 1986; quoted, Howard 1989)

photooxidation $t_{½}$ = 7–71 h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: $t_{½}$ = 168–672 h, based on aerobic river die-away test data (Ludzack et al. 1958; selected value, Howard et al. 1991);

volatilization $t_{½}$ = 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 $t_{½}$ = 1–8 d in freshwater (Howard 1989);

calculated $t_{½}$= 390 h for a body of water with 1 m in depth (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

photooxidation $t_{½}$ = 480 min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: $t_{½}$ = 336–672 h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 10 d in flooded soil (Howard 1989);

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$t_{½}$ = 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 14.1.3.1.1
Reported aqueous solubilities of 2-nitrophenol at various temperatures

Sidgwick et al. 1915		Schwarzenbach et al. 1988		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-UV spec.		shake flask-UV spec		shake flask-optical method	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
		solid					
38.4	3210	0	747	10	895	17.35	1169
42.8	3460	10	898	20	1350	31.35	2434
47.5	3760	20	1080	30	2000	36.85	3144
59.4	4550	30	1457	40	2840	49.55	3951
65.7	5130	for supercooled liquid			17.35	1169	
72.8	5890	0	2058	mp/K	317.95	30.05	2281
80.3	6900	10	1920	ΔH_{fus}/(kJ mol^{-1}) = 17.44		37.55	3186
88.9	8330	20	2011	Enthalpies of solution*:		49.55	3951
109.9	13430	30	1877	ΔH_{sol}(solid) = 28.7 kJ mol^{-1}		17.35	1169
151.8	30300			ΔH_{sol}(liq.) = 11.2 kJ mol^{-1}		31.25	2434
169.5	50400					36.85	3144
196.5	99000					49.55	3951
...	...	Achard et al. 1996					
196.5	906800	shake flask-conductimetry					
163.4	951400	t/°C	S/g·m^{-3}				
91.7	984800						
82.9	987300	15.6	1076				
59.3	992400	24.8	1697				
43.6	995100	34.7	2935				
44.9	1000000						
critical solution temp >200°							
triple point	43.5°C						

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

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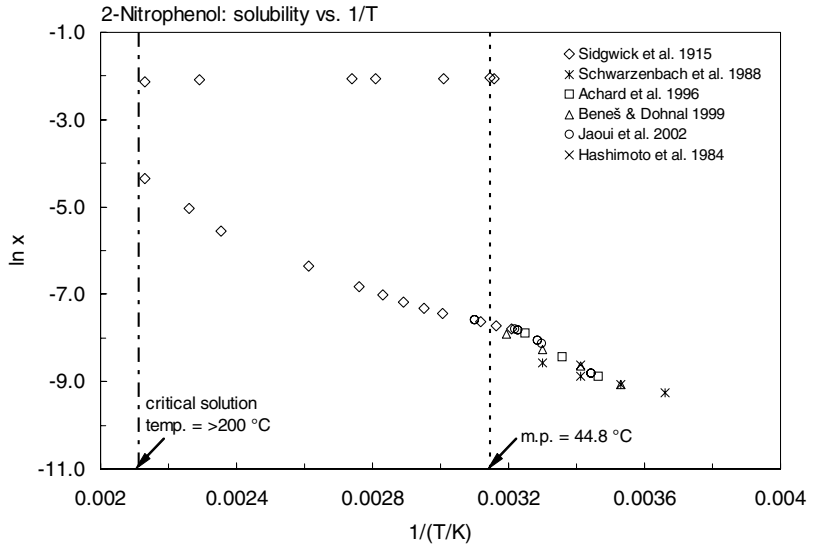

FIGURE 14.1.3.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-nitrophenol.

TABLE 14.1.3.1.2
Reported vapor pressures and Henry's law constants of 2-nitrophenol 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/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Vapor pressure		Henry's law constant			
Stull 1947		Müller & Heal 2001		Harrison et al. 2002	
summary of literature data		gas stripping-UV spec.		gas stripping-UV	
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
			non-equilibrium		
49.3	133	5	0.274	281	0.362
76.8	666.6	10	0.442	284.5	0.396
90.4	1333	15	0.600	289.5	0.607
105.8	2666	20	0.641	293.5	0.930
122.1	5333	25	1.267	298	1.178
132.6	7999	30	1.689	302	1.559
146.4	13332		equilibrium		
167.6	26664	5	0.242	eq. 4	H=/(M atm⁻¹)
191.0	53329	10	0.409	A	–16.6
214.5	101325	15	0.569	B	–6270
		20	0.714		
mp/°C	45	25	1.251		
		30	1.608		
		eq.4	H=/(M atm⁻¹)		
		A	–16.6		
		B	–6290		

For gas-to-liquid transfer
ΔH^{o}/(kJ mol^{-1}) = –52.3 ± 8.1
ΔS^{o}/(J mol^{-1}K^{-1}) = –138 ± 28

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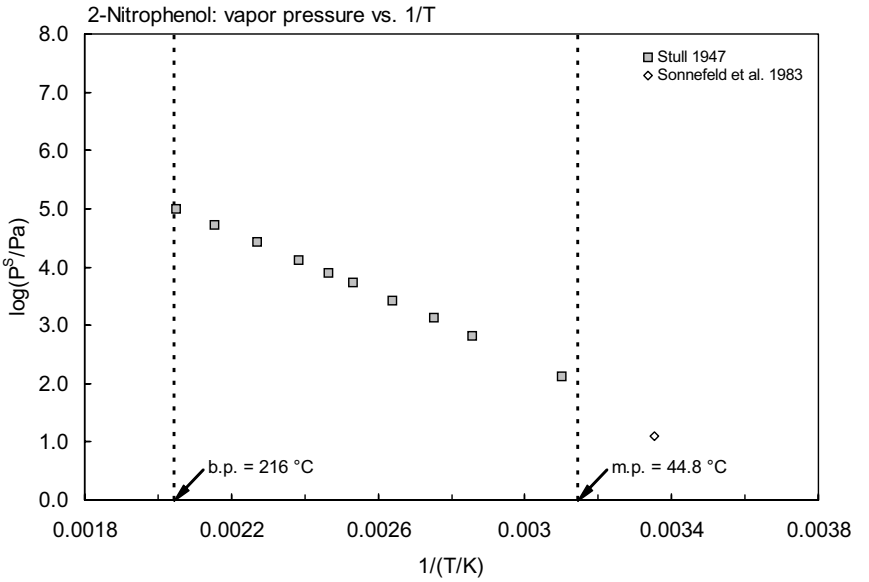

FIGURE 14.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrophenol.

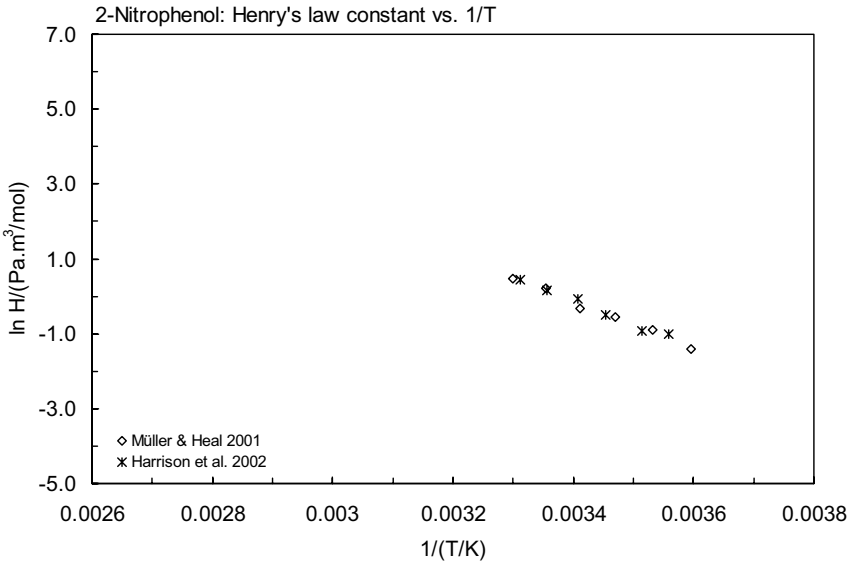

FIGURE 14.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-nitrophenol.

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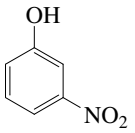
14.1.3.2 3-Nitrophenol



Common Name: 3-Nitrophenol
Synonym: *m*-nitrophenol
Chemical Name: 3-nitrophenol
CAS Registry No: 554-84-7
Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$
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/cm^3 at 20°C):
1.2797 (10°C, Verschueren 1983)
Molar Volume (cm^3/mol):
108.7 (100°C, Stephenson & Malanowski 1987)
131.9 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
8.00 (Fieser & Fieser 1958)
8.36 (Serjeant & Dempsey 1979; Dean 1985; Howard 1989; Haderlein & Schwarzenbach 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.34 (Tsonopoulos & Prausnitz 1971)
19.20 (Beneš & Dohnal 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57.74 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.197 (mp at 96.8°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):
30300* (40.4°C, shake flask-residue volume method, measured range 40.4–98.7°C, critical solution temp 98.7°C, Sidgwick 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 (P_S/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·m^3/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 K_{OW}:
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)

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2.02 (Scherrer & Howard 1979)
1.74 (HPLC-RT correlation, Butte et al. 1981)
2.05 (Beltrame et al. 1988, 1989)
2.01, 2.03 (shake flask, HPLC-RT correlation, Wang et al. 1989)
1.88 (shake flask-UV, Kramer & Henze 1990)
1.74 (centrifugal partition chromatography CPC-RV at pH 7.4, El Tayar et al. 1991)
2.00 (recommended, Sangster 1993)
1.92, 1.51 (COMPUTOX databank, Kaiser 1993)
2.00 (recommended, Hansch et al. 1995)

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, $t_{½}$:

Volatilization: volatilization $t_{½}$ = 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 $t_{½}$ ~ 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 $g^{-1}{\cdot}h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
$t_{½}$ = 6.3 d or less in flooded soil under anaerobic conditions (Howard 1989)
$t_{½}$(aerobic) = 0.76 d, $t_{½}$(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: $t_{½}$ = 14 h for reaction with hydroxyl radical in vapor phase (Howard 1989).
Surface water: $t_{½}$ = 4.2 d in a model river (Howard 1989)
$t_{½}$(aerobic) = 0.76 d, $t_{½}$(anaerobic) = 6.8 d in natural waters (Capel & Larson 1995).
Groundwater:
Sediment:
Soil: $t_{½}$ = 6.3 d in flooded soil under anaerobic conditions (Howard 1989).
Biota: elimination from goldfish within 4 h (Nagel & Urich 1980).

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TABLE 14.1.3.2.1
Reported aqueous solubilities of 3-nitrophenol at various temperatures

Sidgwick et al. 1915						Beneš & Dohnal 1999	
shake flask-synthetic method						shake flask-UV spec	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
40.4	30300	98.5	291000	72.7	673800	10	7200
49.5	36500	98.5	351300	55.8	715600	20	10800
61.1	46600	98.6	388400	42.3	758900	30	16700
67.1	54200	98.7	409400	43.9	793200	40	19000
79.1	76400	98.5	431200	62.0	899000		
85.1	94700	97.9	481200	95.1	1000000	mp/K	369.95
88.5	109400	94.5	539500			ΔH_{fus}/(kJ mol^{-1}) = 19.20	
93.2	139200	91.9	571900	critical solution temp 98.7°C		Enthalpies of solution*:	
97.1	188500	87.3	607400	triple point	41.5°C	ΔH_{sol}(solid) = 29.3 kJ mol^{-1}	
98.0	215500	82.6	634700			ΔH_{sol}(liq.) = 16.1 kJ mol^{-1}	

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

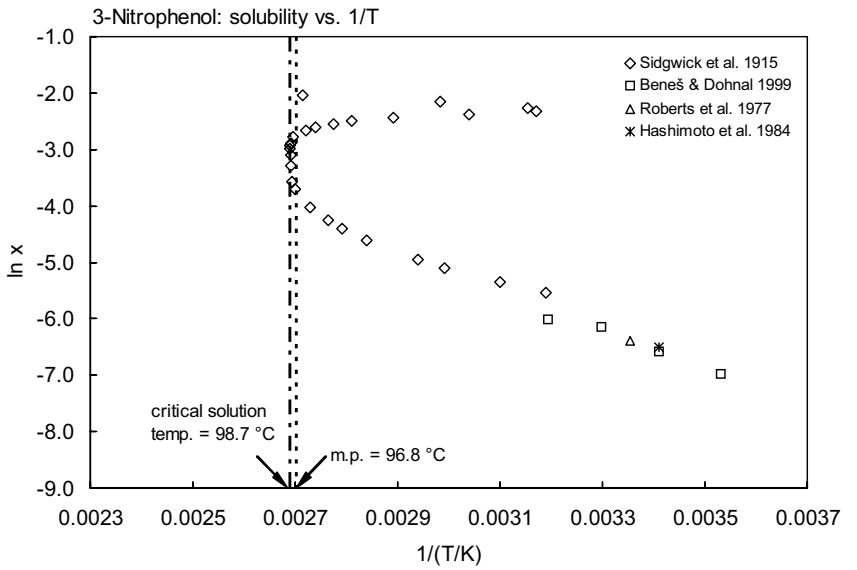

FIGURE 14.1.3.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 3-nitrophenol.

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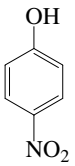
14.1.3.3 4-Nitrophenol



Common Name: 4-Nitrophenol
Synonym: *p*-nitrophenol, 4-hydroxynitrobenzene
Chemical Name: 4-nitrophenol
CAS Registry No: 100-02-7
Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$
Molecular Weight: 139.109
113.6 (Lide 2003)
Boiling Point (°C):
279.0 (decomposes, Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.479 (Weast 1982–83)
Molar Volume (cm^3/mol):
131.9 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
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, ΔH_{fus} (kJ/mol):
15.90 (Tsonopoulos & Prausnitz 1971)
18.25 (Beneš & Dohnal 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
41.09 (Tsonopoulos & Prausnitz 1971)
62.76, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.135 (mp at 113.6°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
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 [S/(mol kg^{-1})] = 17.110 – 4273.4/(T/K); temp range 288–314 K (eq. derived using reported exptl. 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_S/kPa) = 11.9529 – 5159.7/(T/K), temp range 304–352 K (solid, Antoine eq., Stephenson & Malanowski 1987)

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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 ΔS_{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_{OW}:

1.91 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
1.18, 1.27 (calculated-π 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)
1.85, 1.92 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
0.70 (calculated-γ 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_{OW}, Mabey et al. 1982)
0.301 (calculated-K_{OW}, Yoshida et al. 1983)
1.48, 1.45 (alga *chlorella fusca*, wet wt. basis, calculated-K_{OW}, 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_{OC}:

1.65 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.41 (soil, calculated-K_{OW}, 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-MCI χ and fragment contribution, Meylan et al. 1992)

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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, $t_{½}$:

Volatilization:

Photolysis: atmospheric photolysis $t_{½}$ = 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 $t_{½}$ range from hours to a week or more in atmosphere and $t_{½}$ = 2–14 d in clear surface waters (Howard 1989).

Oxidation: oxidation rate constant k < 2×10^5 $M^{-1}{\cdot}h^{-1}$ for singlet oxygen, k = 2×10^6 $M^{-1}{\cdot}h^{-1}$ for peroxy radical (Mabey et al. 1982);
photooxidation $t_{½}$ = 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 $M^{-1}{\cdot}s^{-1}$ 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} $cm^3{\cdot}molecule^{-1}{\cdot}s^{-1}$ for the gas-phase reaction with OH radical at 296 K in the atmosphere (Becker et al. 1984; quoted, Carlier et al. 1986);
photooxidation $t_{½}$ = 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 $t_{½}$ = 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 TiO_2 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 $g^{-1}{\cdot}h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
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 $t_{½}$ = 18.2–168 h, based on pond die-away test data (Paris et al. 1983; Bourquin 1984; selected, Howard et al. 1991);
aqueous anaerobic $t_{½}$ = 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} $mL{\cdot}cell^{-1}{\cdot}h^{-1}$ in water (Mabey et al. 1982);
rate constant of $(3.80 \pm 1.40) \times 10^{-11}$ $L{\cdot}organism^{-1}{\cdot}h^{-1}$ (Paris et al. 1983; quoted, Steen 1991).

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

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 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 $t_{½}$ = 5.7 d at pH 5, $t_{½}$ = 6.7 d at pH 7 and $t_{½}$ = 13.7 d at pH 9 in water (Hustert et al. 1981);
$t_{½}$ = 1–8 d in freshwater, $t_{½}$ = 1–3 yr in marine systems but decreased to 13–20 d with the presence of sediment, the mean $t_{½}$ = 7.7 d estimated by a nonsteady-state equilibrium model, and photolysis $t_{½}$ = 2–14 d in clear surface waters (Howard 1989);
$t_{½}$ = 18.2–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{½}$ = 440 min for photolysis in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

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Groundwater: $t_{½}$ = 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: $t_{½}$ ~ 1 d in agricultural topsoil and $t_{½}$ = 10 d in flooded soil, $t_{½}$ > 40 d in subsoil under aerobic conditions and longer still under anaerobic conditions (Howard 1989);
$t_{½}$ = 17–29 h, based on aerobic soil die-away test data (Loekke 1985; selected, Howard et al. 1998).
$t_{½}$ = 75 d in a coarse sandy soil, $t_{½}$ = 145 d in sandy loam (Kjeldsen et al. 1990)

Biota: depuration $t_{½}$(obs.)= 72 h, $t_{½}$(calc) = 37 h for mean exposure level of 0.0041 μg·mL^{-1} and $t_{½}$(obs.) = 228 h, $t_{½}$(calc) = 206 h for mean exposure level of 0.041 μg·mL^{-1} (Call et al. 1980).

TABLE 14.1.3.3.1
Reported aqueous solubilities of 4-nitrophenol at various temperatures

Sidgwick et al. 1915		Achard et al. 1996		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-conductimetry		shake flask-UV spec.		shake flask-optical method	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
34.8	29100	15.3	10162	10	8050	12.75	8694
37.2	31100	25.0	15599	20	12000	18.15	11477
40.4	33400	30.3	29600	30	17800	23.65	15052
47.7	39300	34.9	28845	38	23900	34.55	25082
51.2	43000					41.05	33428
59.1	53300			mp/K	386.95	14.65	9599
67.8	69900			ΔH_{fus}/(kJ mol^{-1}) = 18.25		19.65	12367
72.6	82800			Enthalpies of solution*:		25.35	16345
79.3	106100	OECD 1981		ΔH_{sol}(solid) = 28.9 kJ mol^{-1}		33.55	23969
84.4	137000	shake flask (6 laboratories)		ΔH_{sol}(liq.) = 16.9 kJ mol^{-1}		39.25	30896
87.9	175300	t/°C	S/g·m^{-3}			11.15	7999
90.2	215800	15	9950†			15.85	10211
91.3	261600	25	14800‡			23.15	14690
92.3	304100.					34.55	25082
92.8	331900	†mean, 8880–10900 g·m^{-3}				40.65	32844
...	...	‡mean, 13800–15900 g·m^{-3}					
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.

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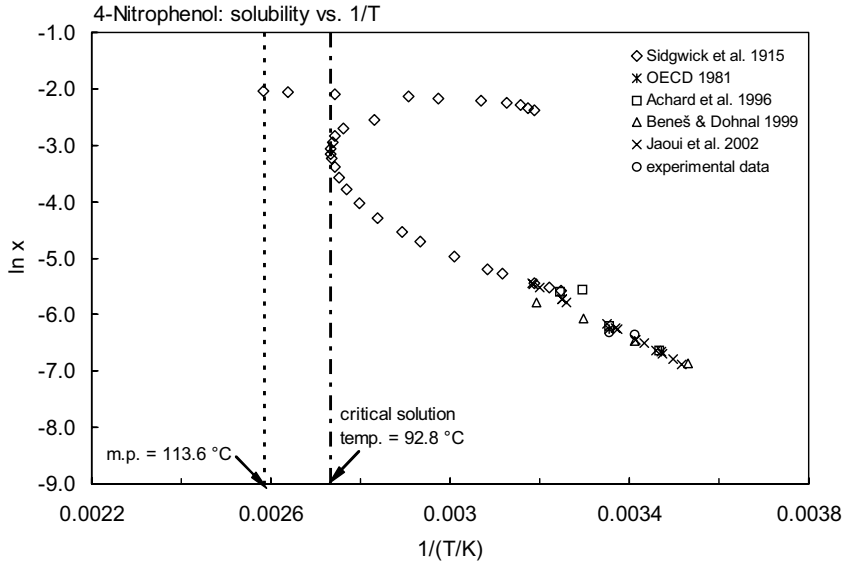

FIGURE 14.1.3.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 4-nitrophenol.

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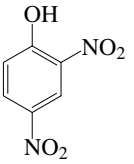
14.1.3.4 2,4-Dinitrophenol



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: $C_6H_4N_2O_5$, $C_6H_3(NO_2)_2OH$
Molecular Weight: 184.106
Melting Point (°C):
114.8 (Lide 2003)
Boiling Point (°C):
sublimation (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.684 (24°C, Weast 1982–83)
Molar Volume (cm^3/mol):
160.4 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
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/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):
6000 (Morrison & Boyd 1959, Howard 1989)
5600 (18°C, Verschueren 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_S/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·m^3/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)

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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, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: aqueous oxidation rate constants $k = 3 \times 10^4$ $M^{-1}\cdot h^{-1}$ for singlet oxygen, and $k = 5 \times 10^5$ $M^{-1}\cdot h^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{½}$ = 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);

photooxidation $t_{½}$ = 111–1114 h in air, based on the estimated reaction rate constant $k = 1.7 \times 10^{-11}$ $cm^3\cdot molecule^{-1}\cdot s^{-1}$ with an ambient hydroxyl radical concentration of 8×10^5 $molecules\cdot cm^{-3}$ for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

aqueous photooxidation $t_{½}$ = 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 $t_{½}$ = 3.6 d in adapted activated sludge under aerobic conditions (Mills et al. 1982);

aqueous aerobic $t_{½}$ = 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 $t_{½}$ = 68–170 h, based on anaerobic flooded soil die-away tests (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

$t_{½}$(aerobic) = 68 d, $t_{½}$(anaerobic) = 2.8 d in natural waters (Capel & Larson 1995)

Biotransformation: bacterial transformation rate constant $k = 3 \times 10^{-9}$ $mL\cdot cell^{-1}\cdot h^{-1}$ 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 $t_{½}$ = 14 h for reaction with photochemically generated OH radical (Howard 1989)

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photooxidation $t_{½}$ = 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 $t_{½}$ = 58 d for reaction with alkylperoxy radical in water (Howard 1989);
$t_{½}$ = 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 $t_{½}$ = 200 min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)
$t_{½}$(aerobic) = 69 d, $t_{½}$(anaerobic) = 2.8 d in natural waters (Capel & Larson 1995)

Groundwater: $t_{½}$ = 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: $t_{½}$ = 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 $t_{½}$ > 50 d in soil (Ryan et al. 1988).
$t_{½}$ = 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/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
solid		supercooled liquid			
5	171.8	0	2019	15.1	415
10	206.6	10	2213	25.0	691
20	335.0	20	2852	35.0	975
30	473.2	30	3199		

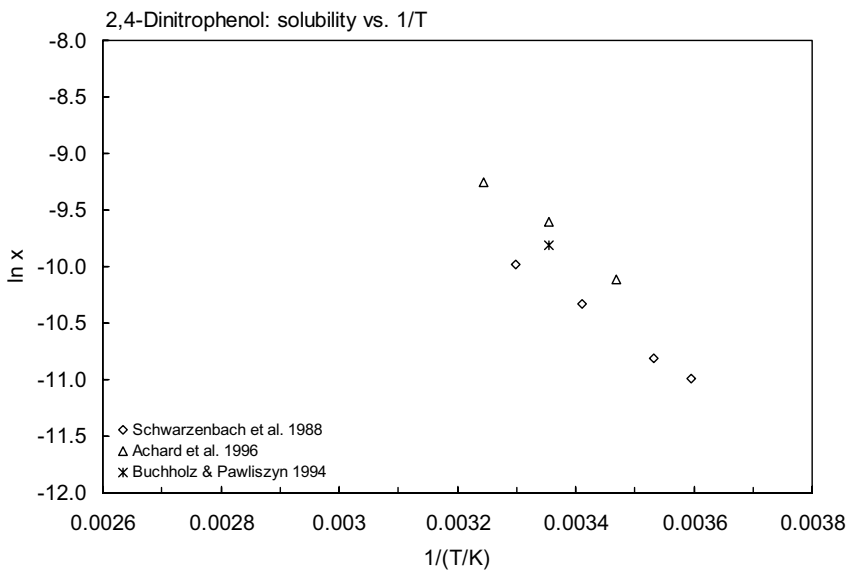

FIGURE 14.1.3.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2,4-dinitrophenol.

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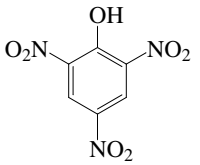
14.1.3.5 2,4,6-Trinitrophenol (Picric acid)



Common Name: 2,4,6-Trinitrophenol
Synonym: Picric acid
Chemical Name: 2,4,6-trinitrophenol
CAS Registry No: 88-89-1
Molecular Formula: $C_6H_3N_3O_7$, $C_6H_2(NO_2)_3OH$
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, ΔH_{fus} (kJ/mol):
19.50 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.37 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{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):
4.68×10^{-5} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/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):
7.66×10^{-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)

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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, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{½}$ = 677–4320 h, based on estimated reaction rates with OH and NO_3 radicals in air (Howard et al. 1991).
Hydrolysis: no hydrolyzable group (Howard et al. 1991).
Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);
aqueous aerobic $t_{½}$ = 672–8640 h, based on aerobic biodegradation screening test (Howard et al. 1991); aqueous anaerobic $t_{½}$ = 48–300 h, based on aqueous anaerobic natural water die-away test data (Howard et al. 1991)
Biotransformation:
Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{½}$ = 672–4320 h, based on estimated photooxidation half-lives in air (Howard et al. 1991).
Surface water: $t_{½}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Ground water: $t_{½}$ = 48–8640 h, based on estimated both aqueous aerobic and aqueous anaerobic biodegradation half-lives (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 672–4320 h, based on estimated photooxidation aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Biota:

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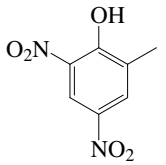
14.1.3.6 4,6-Dinitro-*o*-cresol



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: $C_7H_6N_2O_5$, $CH_3C_6H_2(NO_2)_2OH$
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/cm^3 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 (cm^3/mol):
182.6 (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: 0.249 (mp at 86.5°C)

Water Solubility (g/m^3 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/NaH_2PO_4, 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·m^3/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)

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2.12 (Sangster 1993)
2.56, 1.98 (COMPUTOX databank, Kaiser 1993)

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

Bioconcentration Factor, log BCF:

2.10 (microorganism-water, calculated-K_{OW}, Mabey et al. 1982)
1.38, 1.57 (calculated-S, K_{OW} regression equations., Howard 1991)

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 χ and fragment contribution, Meylan et al. 1992)
3.28 (activated carbon, Blum et al. 1994)

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

Volatilization: nonvolatile from water, based on low Henry's law constant value (Howard 1991).
Photolysis:
Oxidation: aqueous oxidation rate constant $k = 3 \times 10^4$ M^{-1} h^{-1} for singlet oxygen and $k = 5 \times 10^5$ M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);
photooxidation $t_{½}$ = 77–3840 h in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
photooxidation $t_{½}$ = 310–3098 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 $t_{½}$ = 168–504 h, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 68–170 h, based on flooded soil die-away tests for 2,4-dinitrophenol (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)
$t_{½}$(aerobic) = 7 d, $t_{½}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)
Biotransformation: estimated bacterial transformation rate constant $k = 3 \times 10^9$ mL·cell^{-1}·h^{-1} in water (Mabey et al. 1982).
Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 310–3098 h in air, based on estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
$t_{½}$ = 77 d for the vapor-phase reaction with OH radical (concn. of 5×10^5 molecule·cm^{-3}) (Howard 1991); atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).
Surface water: photooxidation $t_{½}$ = of 77–3840 h in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
$t_{½}$ ~ 58 d, estimated for photooxidation via peroxy radicals and $t_{½}$ = 2600 yr for reaction with singlet oxygen in water (Howard 1991)
$t_{½}$(aerobic) = 7 d, $t_{½}$(anaerobic) = 2.8 d in natural waters (Capel & Larson 1995)
Ground water: $t_{½}$ = 68–1008 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 168–504 h, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991).
Biota:

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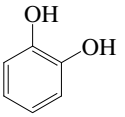
14.1.4 Dihydroxybenzenes, methoxyphenols and chloroguaiacols

14.1.4.1 Catechol (1,2-Dihydroxybenzene)



Common Name: Catechol
Synonym: 1,2-dihydroxybenzene, 1,2-benzenediol, pyrocatechol
Chemical Name: 1,2-dihydroxybenzene
CAS Registry No: 120-80-9
Molecular Formula: $C_6H_4(OH)_2$
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/cm^3):
1.1493 (22°C, Weast 1982–83)
Acid Dissociation Constant, pK_a:
9.40 (Fieser & Fieser 1958)
9.50 (McLeese et al. 1979)
Molar Volume (cm^3/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/m^3 or mg/L at 25°C or as indicated):
71166 (30°C, synthetic method, Walker et al. 1931)
45000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
636190 (quoted, Tsonopoulos & Prausnitz 1971)
35630 (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, Vonterres et al. 1955)
log (P/mmHg) = [–0.2185 × 13779.7/(T/K)] + 8.694319; temp range 104–245.5°C (Antoine eq., Weast 1972–73)
1.34 (extrapolated-Antoine eq., Boublik et al. 1973)
log (P/mmHg) = 7.57299 – 2024.422/(186.533 + t/°C); temp range 118.5–245.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
log (P/mmHg) = [1– 517.477/(T/K)] × 10^{0.902426 – 6.04783 × 10^{-4}·(T/K) + 6.58278 × 10^{-7}·(T/K)^2}; temp range: 377.15–518.65 K, (Cox eq., Chao et al. 1983)
5.44 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.9896 – 3144.241/(281.825 + t/°C); temp range 118.5–245.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.03(extrapolated-Antoine eq., Dean 1985)

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log (P/mmHg) = 7.577 – 2054/(187.0 + t/°C); temp range 118–246°C (Antoine eq., Dean 1985, 1992)
1.06(P_L, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.61028 – 1954.6/(–94.25 + T/K); temp range 395–519y K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/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-k′ 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)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.03 (soil, calculated-MCI $^1\chi$, 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, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: $t_{½} < 2 \times 10^2$ M^{-1} s^{-1} for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{½} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);
photooxidation $t_{½}$ = 2.6–26 h in air, based on vapor-phase reaction rate constant with OH radical in atmosphere (Howard et al. 1991);
aqueous photooxidation $t_{½}$ = 77–3840 h, based on reaction rate constant for RO_2- 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 $Cat_{½}$ in batch culture in 9 d (Schnell et al. 1989);
aqueous aerobic $t_{½}$ = 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 $t_{½}$ = 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: $t_{½}$ = 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: $t_{½}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

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Ground water: $t_{½}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 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

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
104.0	666.6	118.5	1333
118.3	1333	139.3	3333
134.0	2666	157.0	6666
150.6	5333	168.0	9999
161.7	7999	176.2	13332
176.0	13332	188.2	19998
197.7	26664	198.0	26664
221.5	53329	204.0	33330
245.5	101325	210.9	39997
		213.3	43330
mp/°C	105	215.8	46663
		220.0	53329
		224.6	59995
		228.2	66661
		231.4	73327
		235.0	79993
		237.8	86659
		241.0	93325
		245.5	101327
		bp/°C	243.823

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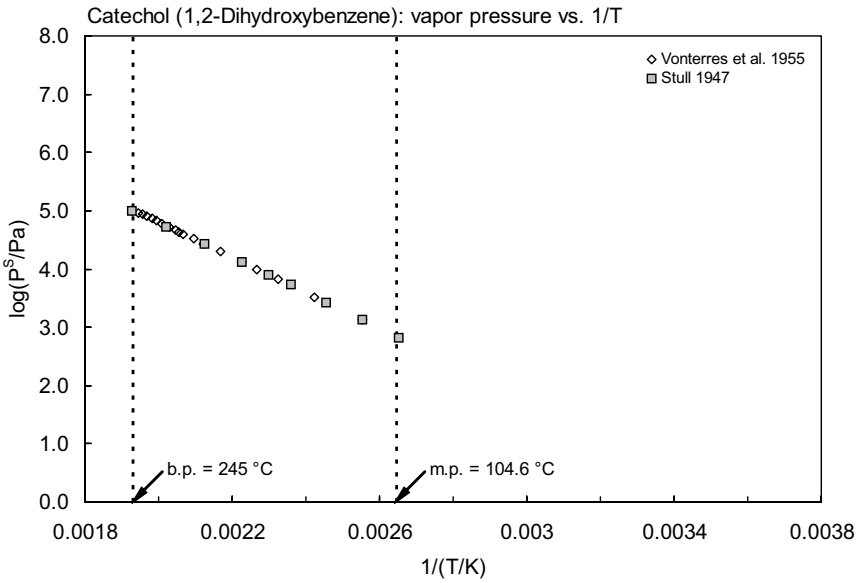

FIGURE 14.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for catechol.

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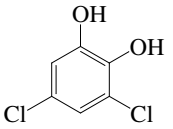
14.1.4.2 3,5-Dichlorocatechol



Common Name: 3,5-Dichlorocatechol
Synonym:
Chemical Name: 3,5-dichlorocatechol
CAS Registry No: 13673-92-2
Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$
Molecular Weight: 179.001
Melting Point (°C):
83–84 (Varhaníčková 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constants, pK_a:
7.78 (Varhaníčková 1995)
Molar Volume (cm^3/mol):
152.6 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
7910 (at pH 4.70. shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at 25°C):

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

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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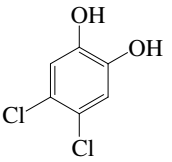
14.1.4.3 4,5-Dichlorocatechol



Common Name: 4,5-Dichlorocatechol
Synonym:
Chemical Name: 4,5-dichlorocatechol
CAS Registry No: 3428-24-8
Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$
Molecular Weight: 179.001
Melting Point (°C):
116–117 (Varhaníčková 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
8.17 (Varhaníčková 1995)
Molar Volume (cm^3/mol):
152.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
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 m^3/mol at 25°C):
0.00078 (calculated-P_L/C_L, Lei et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
2.51–2.93 (NCASI 1992)

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

Bioconcentration Factor, log BCF or log K_B:
1.18–1.51 (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:

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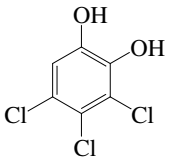
14.1.4.4 3,4,5-Trichlorocatechol



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: $C_6H_3Cl_3O_2$, $C_6HCl_2(OH)_2$
Molecular Weight: 213.446
Melting Point (°C):
130 (Varhaníčková 1995)
134 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a: 6.95 (Varhaníčková 1995)
Molar Volume (cm^3/mol):
173.5 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
79.3 (Lei et al. 1999)
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: 0.085 (mp at 134°C)

Water Solubility (g/m^3 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 P_L, GC-RT correlation, Lei et al. 1999)
$\log (P_L/Pa) = -4135/(T/K) - 12.89$, (GC-RT correlation, Lei et al. 1999)

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

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

Bioconcentration Factor, log BCF or log K_B:
2.16 (estimated-K_{OW}, NCASI 1992)

Sorption Partition Coefficient, log K_{OC}:
4.35 (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, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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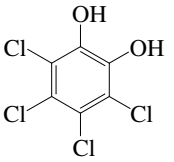
14.1.4.5 Tetrachlorocatechol



Common Name: Tetrachlorocatechol
Synonym: 3,4,5,6-tetrachloro-1,2-benzenediol
Chemical Name: tetrachlorocatechol
CAS Registry No: 1198-55-6
Molecular Formula: $C_6H_2Cl_4O_2$, $C_6Cl_4(OH)_2$
Molecular Weight: 247.891
Melting Point (°C):
194 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
5.83 (Varhaníčková 1995)
Molar Volume (cm^3/mol):
194.4 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.9 (Lei et al. 1999)
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: 0.022 (mp at 194°C)

Water Solubility (g/m^3 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 P_L, GC-RT correlation, Lei et al. 1999)
$\log (P_L/Pa) = -4070/(T/K) - 12.48$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.035 (calculated-P_L/C_L, Lei et al. 1999)

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

Bioconcentration Factor, log BCF or log K_B:
2.54 (estimated-K_{OW}, NCASI 1992)

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Sorption Partition Coefficient, log K_{OC}:

4.56 (sediment, K_P = 36.1 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, $t_{½}$:

Half-Lives in the Environment:

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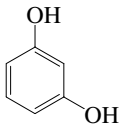
14.1.4.6 Resorcinol (1,3-Dihydroxybenzene)



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: $C_6H_6O_2$, $C_6H_4(OH)_2$
Molecular Weight: 110.111
Melting Point (°C):
109.4 (Lide 2003)
Boiling Point (°C):
276.5 (Lide 2003)
Density (g/cm^3):
1.2717 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
9.40 (Fieser & Fieser 1958; McLeese et al. 1979)
Molar Volume (cm^3/mol):
110.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.30 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55.65 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.149 (mp at 109.4°C)

Water Solubility (g/m^3 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)
1309000 (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, Vonterres 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^{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 (P_S, interpolated-Antoine eq.-I, temp range 10–50°C, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.425 – 4876/(T/K); temp range 283–323 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

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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·m^3/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, $t_{½}$:
Volatilization:
Photolysis: measured pseudo-first-order reaction rate constant k = 0.014 min^{-1} for direct photolysis in aqueous solutions with $t_{½}$ = 50.7 min. (Peijnenburg et al. 1992).
Photooxidation: rate constant k > 3×10^5 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: $t_{½}$ = (50.7 ± 1.0) min for directly photolysis in aqueous solutions (Peijnenburg et al. 1992).
Ground water:
Sediment:
Soil:
Biota:

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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

$\log P = A - B/(T/K)$ (1)
$\log (P/mmHg) = A - B/(C + t/°C)$ (2)
$\log (P/Pa) = A - B/(C + T/K)$ (3)
$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		Vonterres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
					solid
108.4	133.3	151.5	1333	55.35	0.86
138.0	666.6	175.0	3333	66.35	2.73
152.1	1333	190.3	6666	76.45	6.94
168.0	2666	201.7	9999	85.45	14.4
185.3	5333	210.0	13332	92.65	29.2
195.8	7999	221.7	19998	100.05	50.8
209.8	13332	230.1	26664	105.95	81.3
230.8	26664	237.0	33330		
253.4	53329	240.2	39997		
276.5	101325	246.0	43330	eq. 1a	P^S/Pa
		248.0	46663	A	33.807
mp/°C	110.7	252.0	53329	B	11147
		257.0	59995		
		261.0	66661		
		264.0	73327		
		267.0	79993		
		270.0	86659		
		273.0	93325		
		276.5	101325		
		bp/°C	276.205		

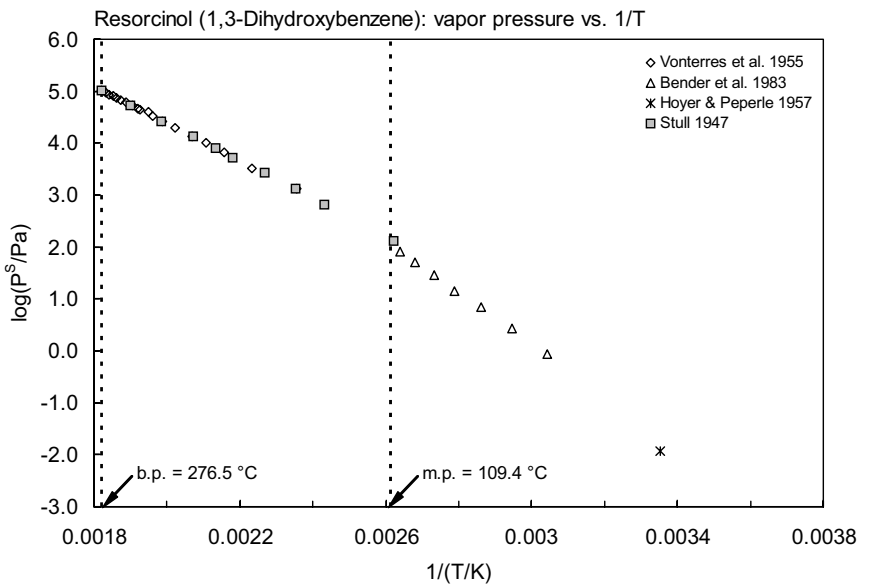

FIGURE 14.1.4.6.1 Logarithm of vapor pressure versus reciprocal temperature for resorcinol.

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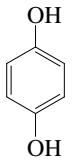
14.1.4.7 Hydroquinone (1,4-Dihydroxybenzene)



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: $C_6H_4(OH)_2$
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, ΔH_{fus} (kJ/mol):
27.11 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
60.67 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{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 (20–25°C, Geyer et al. 1981)
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/mmHg) = [–0.2185 × 18734.0/(T/K)] + 10.309301; temp range 132.4–286.2°C (Antoine eq., Weast 1972–73)
0.00276* (gas saturation, extrapolated - Antoine eq., measured range 68–126°C, Bender et al. 1983)
log (P/mmHg) = [1– 558.031/(T/K)] × 10^{0.941185 – 5.32724 × 10^{-4}·(T/K) + 5.41185 × 10^{-7}·(T/K)^2}; temp range: 432.25–559.15 K, (Cox eq., Chao et al. 1983)
0.03940 (extrapolated - liquid, Antoine eq., Boublik et al. 1984)
log (P/kPa) = 7.41617 – 2397.626/(194.743 + t/°C); temp range 159.1–286°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
0.00255 (P_S, interpolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_S/kPa) = 12.585 – 5420/(T/K); temp range 298–346 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.00575 – 2321.92/(–95.235 + T/K); temp range 448–559 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

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Henry's Law Constant (Pa·m^3/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	(shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
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, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: $k = 1 \times 10^6$ M^{-1} s^{-1} for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{½}$ = 12 min (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2$ M^{-1} s^{-1} for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{½} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);

aqueous photooxidation $t_{½}$ = 0.39–19.3 h in surface water, based on measured rate data for the reaction with alkyl peroxyl radical in aqueous solution (Mill 1982; selected, Howard et al. 1991);

photooxidation $t_{½}$ = 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 $t_{½}$ = 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 $t_{½}$ = 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:

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Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{½}$ = 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 $t_{½}$ = 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: $t_{½}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.4.7.1
Reported vapor pressures of hydroquinone (1,4-dihydroxybenzene) 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/mmHg) = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log (P/Pa) = A – B/(C + T/K)	(3)		
log (P/mmHg) = A – B/(T/K) – C·log (T/K)	(4)		

Stull 1947		Vonterres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
					solid
132.4	133.3*	159.1	1333	67.85	0.46
153.3	666.6*	181.0	3333	79.95	1.70
163.5	1333*	199.1	6666	90.75	4.79
174.6	2666	210.0	9999	100.75	11.2
192.0	5333	218.5	13332	111.25	26.9
203.0	7999	230.1	19998	116.05	40.2
216.5	13332	239.2	26664	121.15	61.1
238.0	26664	246.1	33330	126.45	92.3
262.5	53329	252.0	39997		
286.2	101325	254.8	43330	eq. 1a	P^S/Pa
		257.2	46663	A	35.137
	*solid	259.0	53329	B	12233
mp/°C	170.3	266.1	59995		
		269.5	66661		
		273.0	73327		
		276.7	79993		
		278.8	86659		
		282.0	93325		
		286.0	101325		
		bp/°C	276.17		

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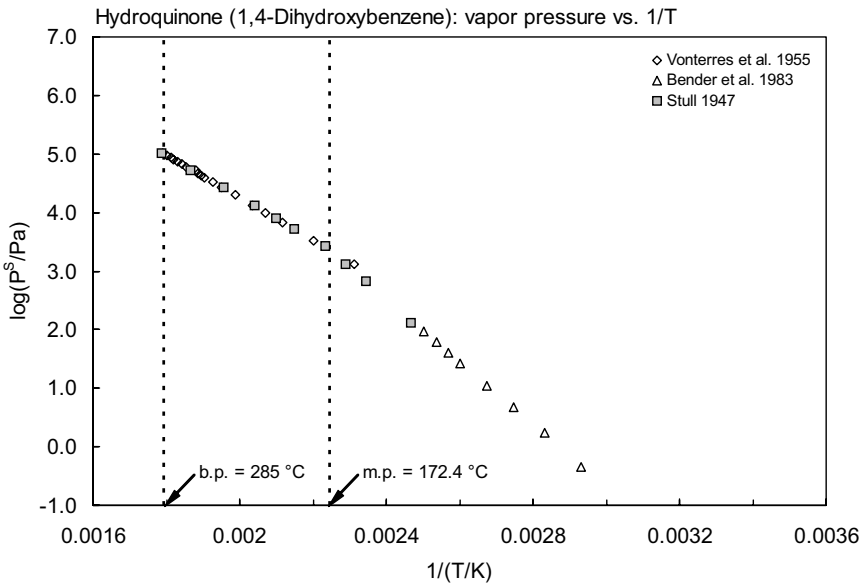

FIGURE 14.1.4.7.1 Logarithm of vapor pressure versus reciprocal temperature for hydroquinone.

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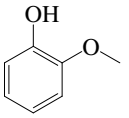
14.1.4.8 2-Methoxyphenol (Guaiacol)



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: $C_7H_8O_2$, $C_6H_4(OCH_3)OH$
Molecular Weight: 124.138
Melting Point (°C):
32 (Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C): 204–206
205 (Lide 2003)
Density (g/cm^3):
1.129 (crystal)
1.112 (liquid, solidified at 28°C)
Acid Dissociation Constant, pK:
Molar Volume (cm^3/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/m^3 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_L/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 m^3/mol at 25°C):
0.30 (calculated-P/C, Sagebiel et al. 1992)

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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 – 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 $^{1}\chi$, Sabljic et al. 1995)

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

Half-Lives in the Environment:

TABLE 14.1.4.8.1
Reported vapor pressures of 2-methoxyphenol (guaiacol) at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
52.4	133.3	82.0	1333
79.1	666.6	102.0	3333
92.0	1333	119.0	6666
106.0	2666	129.5	9999
121.6	5333	136.0	13332
131.0	7999	149.0	19998
144.0	13332	155.5	26664
162.7	26664	164.8	33330
184.1	53329	169.0	39997
205.0	101325	173.0	43330
		175.9	46663
mp/°C	28.5	179.0	53329
		184.7	59995
		187.0	66661
		191.0	73327
		194.0	79993
		198.0	86659
		201.0	93325
		205.0	101325
		bp/°C	204.566

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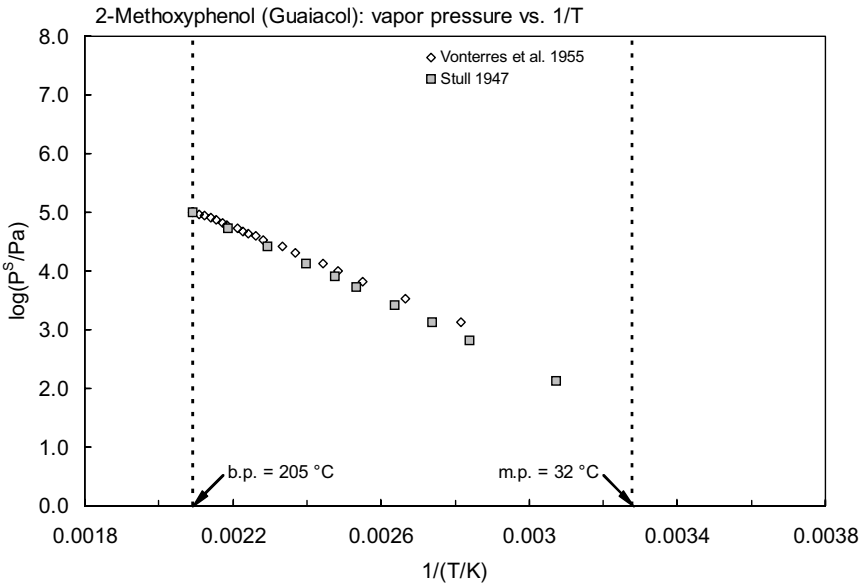

FIGURE 14.1.4.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methoxyphenol (guaiacol).

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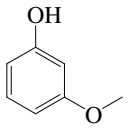
14.1.4.9 3-Methoxyphenol



Common Name: 3-Methoxyphenol
Synonym: *m*-methoxyphenol, *m*-hydroxyanisole, resorcinol monomethylether
Chemical Name: 3-methoxyphenol
CAS Registry No: 150-19-6
Molecular Formula: $CH_3OC_6H_4OH$
Molecular Weight: 124.138
Melting Point (°C):
< –17(Lide 2003)
Boiling Point (°C):
244 (Stephenson & Malanowski 1987)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/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/m^3 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_L/kPa) = 6.12536 – 1572.51/(–136.16 + T/K); temp range 413–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa-m^3/mol at 25°C):
0.10 (estimated as per Sagebiel et al. 1992 data on 2-methoxyphenol)

Octanol/Water Partition Coefficient, log K_{OW}:
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 $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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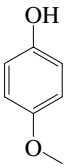
14.1.4.10 4-Methoxyphenol



Common Name: 4-Methoxyphenol
Synonym: *p*-methoxyphenol, *p*-hydroxyanisole, hydroquinone monomethylether
Chemical Name: 4-methoxyphenol
CAS Registry No: 150-76-5
Molecular Formula: $CH_3OC_6H_4OH$
Molecular Weight: 124.138
Melting Point (°C):
57 (Lide 2003)
Boiling Point (°C):
243 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/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/m^3 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_L/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_L, GC-RT correlation, Lei et al. 1999)
log (P_L/Pa) = –3664/(T/K) + 12.28 (GC-RT correlation, Lei et al. 1999)
1.05 (supercooled liquid P_L, calculated-group contribution, Lee et al. 2000)

Henry's Law Constant (Pa·m^3/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}:

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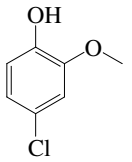
14.1.4.11 4-Chloroguaiacol



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/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/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/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):
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)
4856* (19°C, shake flask-HPLC/UV, measured range 10–50°C, Larachi et al. 2000)
5132; 13200, 10500 (quoted exptl.; calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/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}:

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TABLE 14.1.4.11.1
Reported aqueous solubilities of 4-chloroguaiacol at various temperatures

Larachi et al. 2000	
shake flask-HPLC/UV	
t/°C	S/g·m^{-3}
10.0	4395
11.0	4467
15.0	4548
19.0	4856
36.3	5406
41.0	6658
50.0	6213
54.5	7054
66.0	7040
70.5	8639
78.0	9171
85.6	9540
90.0	10255

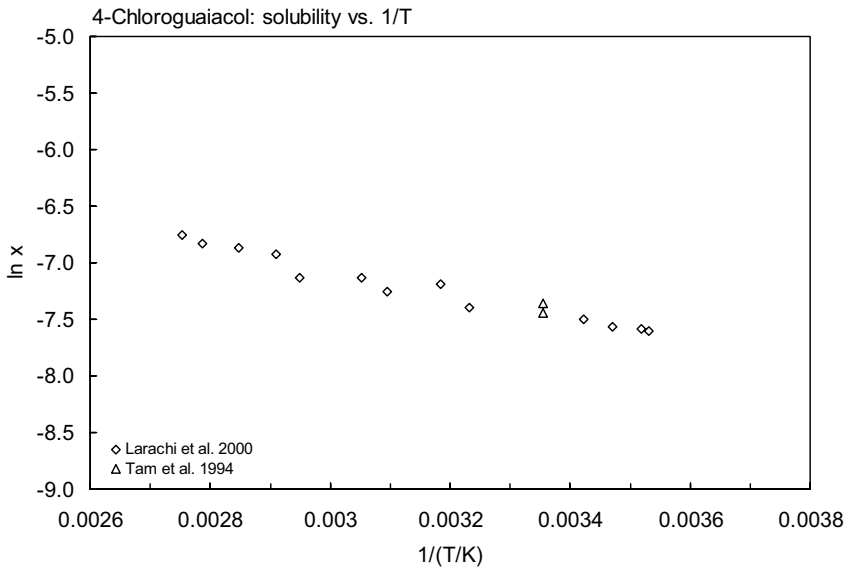

FIGURE 14.1.4.11.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 4-chloroguaiacol.

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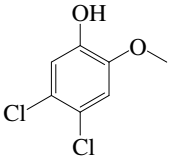
14.1.4.12 4,5-Dichloroguaiacol



Common Name: 4,5-Dichloroguaiacol
Synonym: 4,5-dichloro-2-methoxyphenol
Chemical Name: 4,5-dichloroguaiacol
CAS Registry No: 2460-49-3
Molecular Formula: $C_7H_6Cl_2O_2$
Molecular Weight: 193.028
Melting Point (°C): 69–70
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
8.26, 8.52 (20°C, regressions, Xie & Dyrssen 1984)
Molar Volume (cm^3/mol):
176.5 (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:

Water Solubility (g/m^3 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 P_L, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.44 (calculated-P_L/C_L, Lei et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
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 & Dryssen 1984)
3.26 (recommended, Sangster 1993)

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

Bioconcentration Factor, log BCF or log K_B:
1.74–2.05, 2.03 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
1.18–1.51, 1.75 (quoted, estimated, NCASI 1992)
2.03 (*Oncorhynhus mykiss*, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

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:

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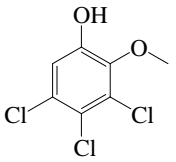
14.1.4.13 3,4,5-Trichloroguaiacol



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: $C_7H_5Cl_3O_2$
Molecular Weight: 227.473
Melting Point (°C): 85–86
Boiling Point (°C):
Density (g/cm^3):
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 (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 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·m^3/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)

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Sorption coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Biota: $t_{½}$ = 1–2 d in bleak and $t_{½}$ = 2 d in trout (Niimi et al. 1990).

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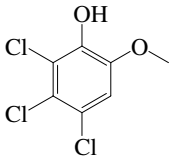
14.1.4.14 4,5,6-Trichloroguaiacol



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: $C_7H_5Cl_3O_2$
Molecular Weight: 227.473
Melting Point (°C): 112–115
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:

7.07 (Leuenberger et al. 1985)
7.20 (20°C, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^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^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_{OW}:

3.74 (shake flask-GC, Xie et al. 1984)
3.92, 3.91, 3.78 (HPLC-k′ correlation, calculated-π const., calculated-f const., Xie et al. 1984)
3.73, 3.74. 3.72 (shake flask-GC, regressions, Xie & Dyrssen 1984)
3.57 (calculated-fragment const., Niimi et al. 1990)
3.72, 3.92 (literature values, Sangster 1993)
3.82 (COMPUTOX databank, Kaiser 1993)
3.72, 3.92 (literature values, Hansch et al. 1995)
3.19 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{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)

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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 χ 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, $t_{½}$:

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: $t_{½}$ = 1 to 2 d in bleak (Niimi et al. 1990).

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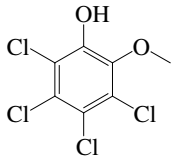
14.1.4.15 3,4,5,6-Tetrachloroguaiacol



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: $C_7H_4Cl_4O_2$
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, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
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_{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_{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)

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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 χ, Bahnick & Doucette 1988)
2.85, 3.17 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.85 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

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: $t_{½}$ < 10 d in trout liver (Niimi et al. 1990); $t_{½}$ = 1–2 d in bleak (Niimi et al. 1990).

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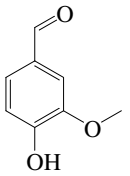
14.1.4.16 Vanillin (4-Hydroxy-3-methoxybenzaldehyde)



Common Name: Vanillin
Synonym: 4-hydroxy-3-methoxybenzaldehyde, vanillic aldehyde, methylprotocatechuic aldehyde
Chemical Name: 4-hydroxy-3-methoxybenzaldehyde
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/cm^3):
1.056 (Weast 1982–83)
Acid Dissociation Constant, pK_a:
7.40 (Sangster 1993)
7.62 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
156.9 (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: 0.279 (mp at 81.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2480 (at pH 4.50, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at 25°Cor as indicated and reported temperature dependence equations):
133.3 (107°C, summary of literature data, temp range 107–285°C, Stull 1947)
log (P_S/kPa) = 10.997 – 4623/(T/K); temp range 288–333 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 10.93562 – 4535.023/(T/K); temp range 297–328 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.01734 – 3198.18/(–17.047 + T/K); temp range 380–558 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = $-25.583 - 4.086 \times 10^3/(T/K) + 17.515 \cdot \log (T/K) - 2.8177 \times 10^{-2} \cdot (T/K) + 1.0912 \times 10^{-5} \cdot (T/K)^2$; temp range 355–777 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/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)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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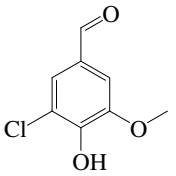
14.1.4.17 5-Chlorovanillin



Common Name: 5-Chlorovanillin
Synonym:
Chemical Name: 5-chlorovanillin
CAS Registry No: 19463-48-0
Molecular Formula: $C_8H_7ClO_3$, $C_6H_2ClCHO(OCH_3)$
Molecular Weight: 185.593
Melting Point (°C):
165 (Weast 1982–83; Lide 2003)
169 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a
6.80 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
177.8 (Le Bas method -calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.042 (mp at 165°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):
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 m^3/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:

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TABLE 14.1.4.17.1
Reported aqueous solubilities of 5-chlorovanillin at various temperatures

Larachi et al. 2000	
shake flask-HPLC/UV	
t/°C	S/g·m^{-3}
7.5	171
12.0	171
16.8	184
19.8	168
24.0	249
30.0	286
36.5	505
46.0	629
50.0	760
59.0	932
65.0	1139
70.0	1267
80.0	1767
85.9	2314

ΔS_{fus}/(kJ mol^{-1}) = 89.1

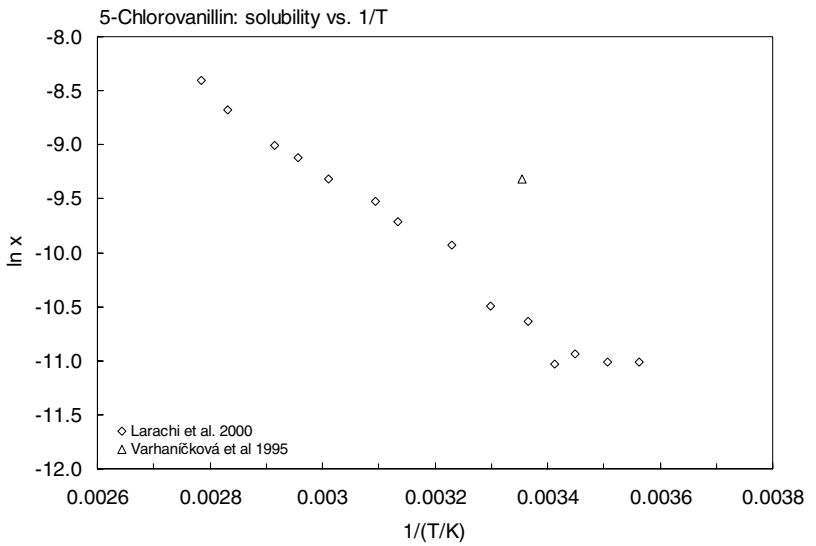

FIGURE 14.1.4.17.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 5-chlorovanillin.

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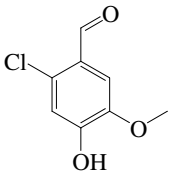
14.1.4.18 6-Chlorovanillin



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/cm^3):
Acid Dissociation Constant, pK_a:
6.11 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
177.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
132 (at pH 5.35, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/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:

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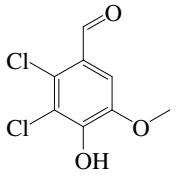
14.1.4.19 5,6-Dichlorovanillin



Common Name: 5,6-Dichlorovanillin
Synonym:
Chemical Name: 5,6-dichlorovanillin
CAS Registry No: 18268-69-4
Molecular Formula: $C_8H_6Cl_2O_3$, $C_6HCl_2CHO(OCH_3)$
Molecular Weight: 221.038
Melting Point (°C):
198–199 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
5.28 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
198.7 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
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 m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
2.47 (NCASI 1992)

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

Bioconcentration Factor, log BCF or log K_B:
1.76 (estimated, K_{OW}, NCASI 1996)

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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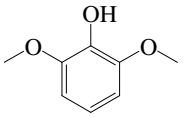
14.1.4.20 Syringol (2,6-Dimethoxyphenol)



Common Name: Syringol
Synonym: 2,6-dimethoxyphenol
Chemical Name: 2,6-dimethoxyphenol
CAS Registry No: 91-10-1
Molecular Formula: $C_8H_{10}O_3$, $C_6H_3OH(OCH_3)_2$
Molecular Weight: 154.163
Melting Point (°C):
53–56 (Aldrich catalog 1998–1999)
56.5 (Lide 2003)
Boiling Point (°C):
261 (Aldrich catalog 1998–1999; Lide 2003)
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
166.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
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 m^3/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)
1.15 (recommended, Sangster 1993)
1.15 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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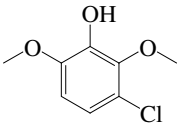
14.1.4.21 3-Chlorosyringol



Common Name: 3-Chlorosyringol
Synonym: 3-chloro-2,6-dimethoxyphenol
Chemical Name: 3-chlorosyringol
CAS Registry No: 18113-22-9
Molecular Formula: $C_8H_9ClO_3$, $C_6H_2(OH)Cl(OCH_3)_2$
Molecular Weight: 188.608
Melting Point (°C):
35-36 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
9.09 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
186.9 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
68.6 (Lei et al. 1999)
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/m^3 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 P_L, GC-RT correlation, Lei et al. 1999)
$\log (P_L/Pa) = -3580/(T/K) - 11.93$ (GC-RT correlation, Lei et al. 2001)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.011 (calculated-P_L/C_L, Lei et al. 1999)

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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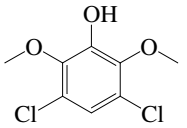
14.1.4.22 3,5-Dichlorosyringol



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: $C_8H_8Cl_2O_2$, $C_6H(OH)Cl_2(OCH_3)_2$
Molecular Weight: 223.054
Melting Point (°C):
105–106 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constants, pK_a:
7.27 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
207.8 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
70.4 (Lei et al. 1999)
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/m^3 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 P_L, GC-RT correlation, Lei et al. 1999)
log (P_L/Pa) = –3679/(T/K) – 12.01, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.069 (calculated-P_L/C_L, Lei et al. 1999)

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

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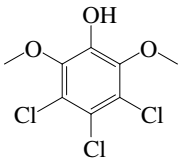
14.1.4.23 Trichlorosyringol



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: $C_8H_7Cl_3O_3$, $C_6(OH)Cl_3(OCH_3)_2$
Molecular Weight: 257.499
Melting Point (°C):
122–123 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
7.73 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
228.7 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.4 (Lei et al. 1999)
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/m^3 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 P_L, GC-RT correlation; Lei et al. 1999)
$\log (P_L/Pa) = -4014/(T/K) - 12.44$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.022 (calculated-P_L/C_L, Lei et al. 1999)

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

Bioconcentration Factor, log BCF or log K_B:
1.19 (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:

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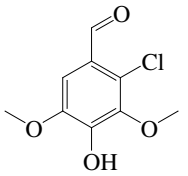
14.1.4.24 2-Chlorosyringaldehyde



Common Name: 2-Chlorosyringaldehyde
Synonym:
Chemical Name: 2-chlorosyringaldehyde
CAS Registry No: 76341-69-0
Molecular Formula: $C_9H_9ClO_4$, $C_6H(OH)Cl(CHO)(OCH_3)_2$
Molecular Weight: 216.619
Melting Point (°C):
196–197 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
6.80 (Varhaníčková et al 1995)
Molar Volume (cm^3/mol):
209.1 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.7 (Lei et al. 1999)
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/m^3 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 P_L, GC-RT correlation; Lei et al. 1999)
$\log (P_L/Pa) = -4058/(T/K) - 12.51$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.069 (calculated-P_L/C_L, Lei et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.81 (quoted, NCASI 1992)

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

Bioconcentration Factor, log BCF or log K_B:
0.62 (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:

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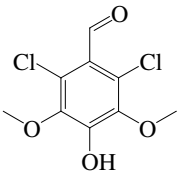
14.1.4.25 2,6-Dichlorosyringaldehyde



Common Name: 2,6-Dichlorosyringaldehyde
Synonym:
Chemical Name:
CAS Registry No: 76330-06-8
Molecular Formula: $C_9H_8Cl_2O_4$, $C_6(OH)Cl_2(CHO)(OCH_3)_2$
Molecular Weight: 251.064
Melting Point (°C):
195.6 (Varhaníčková et al 1995)
Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
230.0 (Le Bas method-calculated at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
82.2 (Lei et al. 1999)
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/m^3 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 P_L, GC-RT correlation; Lei et al. 1999)
log (P_L/Pa) = –4293/(T/K) – 12.79, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.0037 (calculated-P_L/C_L, Lei et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
2.52 (quoted, NCASI 1992)

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

Bioconcentration Factor, log BCF or log K_B:
1.19 (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:

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TABLE 14.2.1
Summary of physical properties of phenolic compounds

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol		pK_a
							MW/ ρ at 20°C	Le Bas	
Alkylphenols and other substituted phenols:									
Phenol	108-95-2	C_6H_5OH	94.111	40.89	181.87	0.698	88.99	103.4	9.89
o-Cresol (2-Methylphenol)	95-48-7	$C_6H_4(CH_3)OH$	108.138	31.03	191.04	0.873	105.26	125.6	10.26
m-Cresol (3-Methylphenol)	108-39-4	$C_6H_4(CH_3)OH$	108.138	12.24	202.27	1	104.62	125.6	10
p-Cresol (4-Methylphenol)	106-44-5	$C_6H_4(CH_3)OH$	108.138	34.77	201.98	0.802	106.25	125.6	10.26
2,6-Di-*t*-butyl-4-methylphenol	128-37-0	$C_{15}H_{24}O$	220.351	71	265	0.354		303.2	
2,3-Dimethylphenol	526-75-0	$C_8H_{10}O$	122.164	72.5	216.9	0.342		147.8	
2,4-Dimethylphenol	105-67-9	$C_8H_{10}O$	122.164	24.5	210.98	1		147.8	10.6
2,5-Dimethylphenol	98-87-4	$C_8H_{10}O$	122.164	74.8	211.1	0.325		147.8	10.3
2,6-Dimethylphenol	576-26-1	$C_8H_{10}O$	122.164	45.8	201.07	0.625		147.8	10.6
3,4-Dimethylphenol	95-65-8	$C_8H_{10}O$	122.164	65.1	227	0.404	124.28	147.8	10.4
3,5-Dimethylphenol	108-68-9	$C_8H_{10}O$	122.164	63.4	221.74	0.420		147.8	10.2
2,3,5-Trimethylphenol	697-82-5	$C_9H_{12}O$	136.190	94.5	233	0.208		170.0	10.6
2,3,6-Trimethylphenol	2416-94-6	$C_9H_{12}O$	136.190	63		0.424		170.0	
2,4,5-Trimethylphenol	496-78-6	$C_9H_{12}O$	136.190	72	232	0.346		170.0	
2,4,6-Trimethylphenol	527-60-6	$C_9H_{12}O$	136.190	73	220	0.338		170.0	10.9
3,4,5-Trimethylphenol	527-54-8	$C_9H_{12}O$	136.190	108	248.5	0.153		170.0	
3-Methyl-5-ethylphenol		$C_9H_{12}O$	136.190					170.0	10.1
o-Ethylphenol	90-00-6	$C_8H_{10}O$	122.164	18	204.5	1		147.8	
m-Ethylphenol	620-17-7	$C_8H_{10}O$	122.164	–4	218.4	1		147.8	
p-Ethylphenol	123-07-9	$C_8H_{10}O$	122.164	45	217.9	0.636		147.8	
2-Propylphenol	644-35-9	$C_9H_{12}O$	136.190	7	220	1		170.0	
4-Propylphenol	645-56-7	$C_9H_{12}O$	136.190	22	232.6	1	134.98	170.0	10.3
2-Isopropylpheonol	88-69-7	$C_9H_{12}O$	136.190	15.5	213.5	1		170.0	
4-Isopropylphenol	99–89–8	$C_9H_{12}O$	136.190	62.3	230	0.431		170.0	10.3
4-Butylphenol	1638-22-8	$C_{10}H_{14}O$	150.217	22	248	1		192.2	10.3
2-*sec*-Butylphenol	89–72–5	$C_{10}H_{14}O$	150.217	16	228	1		192.2	
2-*tert*-Butylphenol	88-18-6	$C_{10}H_{14}O$	150.217	B6.8	223	1		192.2	

(Continued)

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TABLE 14.2.1 *(Continued)*

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol		pK_a
							MW/ ρ at 20°C	Le Bas	
3-*tert*-Butylphenol	585-34-2	$C_{10}H_{14}O$	150.217	42.3	240	0.676		192.2	10.1
4-*sec*-Butylphenol	99-71-8	$C_{10}H_{14}O$	150.217	61.5	241	0.438		192.2	
4-*tert*-Butylphenol	98-54-4	$C_{10}H_{14}O$	150.217	98	237	0.192		192.2	9.9
2-Methyl-5-*tert*-butylphenol		$C_{11}H_{16}O$	164.244					214.4	
2,6-Di-*sec*-butylphenol	128–39–2	$C_{14}H_{22}O$	206.324	39		0.729		281.0	
3,5-Di-*tert*-butylphenol	1138–52–9	$C_{14}H_{22}O$	206.323	88		0.241		281.0	
3-Pentylphenol		$C_{11}H_{16}O$	164.244					214.4	
4-Hexylphenol	2446–69–7	$C_{12}H_{18}O$	178.270	32		0.854		236.6	
2-Heptylphenol		$C_{13}H_{20}O$	192.297					258.8	
4-Heptylphenol	1987–50–4	$C_{13}H_{20}O$	192.297					258.8	
4-Octylphenol	1806–26–4	$C_{14}H_{22}O$	206.324	43		0.666		281.0	
4-*tert*-Octylphenol	140–66–9	$C_{14}H_{22}O$	206.324	85.8	279	0.253		281.0	
4-Nonylphenol	104-40-5	$C_{15}H_{24}O$	220.351	42	approx. 295	0.681		303.2	
1-Naphthol	90-15-3	$C_{10}H_8O$	144.170	95	288	0.206		155.0	
2-Naphthol	135-19-3	$C_{10}H_8O$	144.170	121.5	285	0.113	112.63	155.0	
2-Phenylphenol (2-Hydroxybiphenyl)	90-43-7	$C_{12}H_{10}O$	170.206	57.5	286	0.480		192.0	
3-Phenylphenol (3-Hydroxybiphenyl)	588-51-8	$C_{12}H_{10}O$	170.206	78	>300	0.302		192.0	
4-Phenylphenol (4-Hydroxybiphenyl)	92-69-3	$C_{12}H_{10}O$	170.206	166	305	0.0414		192.0	
2-Allylphenol	1745-81-9	$C_9H_{10}O$	134.174	B6	220	1		162.6	
Chlorophenols:									
2-Chlorophenol	95-57-8	C_6H_4OHCl	128.556	9.4	174.9	1	101.75	124.3	8.49
3-Chlorophenol	108-43-0	C_6H_4OHCl	128.556	32.6	214	0.842		124.3	8.85
4-Chlorophenol	106-48-9	C_6H_4OHCl	128.556	42.8	220	0.669	101.62	124.3	9.18
2,3-Dichlorophenol	576-24-9	$C_6H_4Cl_2O$	163.001	58	206	0.474		145.2	6.44
2,4-Dichlorophenol	120-83-2	$C_6H_4Cl_2O$	163.001	45	210	0.636		145.2	7.68
2,5-Dichlorophenol	583-78-8	$C_6H_4Cl_2O$	163.001	59	211	0.464		145.2	6.45
2,6-Dichlorophenol	87-65-0	$C_6H_4Cl_2O$	163.001	68.5	220	0.374		145.2	6.8
3,4-Dichlorophenol	95-77-2	$C_6H_4Cl_2O$	163.001	68	253	0.379		145.2	7.39
3,5-Dichlorophenol	591-35-5	$C_6H_4Cl_2O$	163.001	68	233	0.379		145.2	6.92
2,3,4-Trichlorophenol	15950-66-0	$C_6H_3Cl_3O$	197.446	83.5	sublim	0.267		166.1	7.66
2,3,5-Trichlorophenol	933-78-8	$C_6H_3Cl_3O$	197.446	62		0.433		166.1	7.37
2,3,6-Trichlorophenol	933-75-5	$C_6H_3Cl_3O$	197.446	58		0.474		166.1	7.13
2,4,5-Trichlorophenol	95-95-4	$C_6H_3Cl_3O$	197.446	69	247	0.370		166.1	7.43

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2,4,6-Trichlorophenol	88-06-2	$C_6H_3Cl_3O$	197.446	69	246	0.370		166.1	7.42
3,4,5-Trichlorophenol	609-19-8	$C_6H_3Cl_3O$	197.446	101	275	0.180		166.1	7.74
2,3,4,5-Tetrachlorophenol	4901-51-3	$C_6H_2Cl_4O$	231.891	116.5	sublim	0.127		187.0	6.96
2,3,4,6-Tetrachlorophenol	58-90-3	$C_6H_2Cl_4O$	231.891	70		0.362		187.0	5.38
2,3,5,6-Tetrachlorophenol	935-95-5	$C_6H_2Cl_4O$	231.891	115		0.131		187.0	5.48
Pentachlorophenol	87-86-5	C_6HCl_5O	266.336	174	310 dec	0.0345		207.9	4.92
4-Chloro-*m*-cresol	59–50–7	C_7H_7ClO	142.583	67	235	0.387		146.5	
Nitrophenols:									
2-Nitrophenol	88-75-5	$C_6H_4OHNO_2$	139.109	44.8	216	0.639		131.9	7.23
3-Nitrophenol	554-84-7	$C_6H_4OHNO_2$	139.109	96.8		0.197		131.9	8.36
4-Nitrophenol	100-02-7	$C_6H_4OHNO_2$	139.109	113.6	279	0.135	94.06	131.9	7.08
2,4-Dinitrophenol	51-28-5	$C_6H_4N_2O_5$	184.106	114.8	sublim	0.132		160.4	4.09
2,6-Dinitrophenol	329-71-5	$C_6H_4N_2O_5$	184.106	108		0.153		160.4	
2,4,6-Trinitrophenol (Picric acid)	88-89-1	$C_6H_3N_3O_7$	229.104	122.5	300 exp	0.111		188.9	0.8
4,6-Dinitro-*o*-cresol	534-52-1	$C_7H_6N_2O_5$	198.133	86.5		0.249		182.6	4.35
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:									
Catechol (1,2-Dihydroxybenzenene)	120-80-9	$C_6H_4(OH)_2$	110.111	104.6	245	0.166		110.8	9.5
3,5-Dichlorocatechol	13673-9-2	$C_6H_2Cl_2(OH)_2$	179.001	83–84		0.267		152.6	7.78
4,5-Dichlorocatechol	3428-24-8	$C_6H_2Cl_2(OH)_2$	179.001	116-117		0.127		152.6	
3,4,5-Trichlorocatechol	56961-20-7	$C_6HCl_3(OH)_2$	213.446	134		0.0850		173.5	6.95
Tetrachlorocatechol	1198-55-6	$C_6Cl_4(OH)_2$	247.891	194		0.0220		194.4	5.83
Resorcinol (1,3-Dihydroxybenzene)	108-46-3	$C_6H_4(OH)_2$	110.111	109.4	276.5	0.149		110.8	9.4
Hydroquinone (1,4-Dihydroxybenzene)	123-31-9	$C_6H_4(OH)_2$	110.111	172.4	285	0.0358		110.8	
2-Methoxyphenol (Guaiacol)	90-05-1	$C_7H_8O_2$	124.138	32	205	0.854		134.7	
3-Methoxyphenol	150-19-6	$C_7H_8O_2$	124.138	< B17	244	1		134.7	
4-Methoxyphenol	150-76-5	$C_7H_8O_2$	124.138	57	243	0.485		134.7	
4-Chloroguaiacol	16766-30-6	$C_7H_7ClO_2$	158.582	liquid		1		155.6	
5-Chloroguaiacol	3753-23-5	$C_7H_7ClO_2$	158.582	34-35		0.807		155.6	
4,5-Dichloroguaiacol	2460-49-3	$C_7H_6Cl_2O_2$	193.028	69-79		0.331		176.5	8.52
4,6-Dichloroguaiacol	2460-49-3	$C_7H_6Cl_2O_2$	193.028	63-64		0.419		176.5	
3,4,5-Trichloroguaiacol	57057-83-7	$C_7H_5Cl_3O_2$	227.473	85-86		0.255		197.4	7.56
4,5,6-Trichloroguaiacol	2668-24-8	$C_7H_5Cl_3O_2$	227.473	112-115		0.137		197.4	7.2
Tetrachloroguaiacol	2539-17-5	$C_7H_4Cl_4O_2$	261.918	121-122		0.113		218.3	6.26
Vanillin	121-33-5	$C_8H_8O_3$	152.148	81.5	285	0.279		156.9	7.42
5-Chlorovanillin	19463-48-0	$C_8H_7ClO_3$	185.593	165		0.0423		177.8	6.80
6-Chlorovanillin	18268-69-4	$C_8H_7ClO_3$	185.593	171–172		0.0365		177.8	6.11

(Continued)

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TABLE 14.2.1 *(Continued)*

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol		pK_a
							MW/ ρ at 20°C	Le Bas	
5,6-Dichlorovanillin	18113–22–9	$C_8H_6Cl_2O_3$	221.038	198–199		0.0198		198.7	5.28
Syringol (2,6-Dimethoxyphenol)	91–10–1	$C_8H_{10}O_3$	154.163	56.5	261	0.491		166.0	
3-Chlorosyringol	18113–22–9	$C_8H_9ClO_3$	188.608	35–36		0.789		186.9	9.09
3,5-Dichlorosyringol	78782–46–4	$C_8H_8Cl_2O_3$	223.054	105–106		0.162		207.8	7.27
Trichlorosyringol	2539–26–6	$C_8H_7Cl_3O_3$	257.499	122–123		0.111		228.7	7.73
2-Chlorosyringaldehyde	76341–69–0	$C_9H_9ClO_4$	216.619	196–197		0.0208		209.1	6.80
2,6-Dichlorosyringaldehyde	76330–06–8	$C_9H_8Cl_2O_4$	251.064	195.6		0.0212		230.0	

* Assuming ΔS_{fus} = 56 J/mol K.

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TABLE 14.2.2
Summary of selected physical-chemical properties of phenolic compounds at 25°C

Compound	Selected properties: Vapor pressure P_S/Pa	Vapor pressure P_L/Pa	Solubility S/(g/m³)	Solubility C^S/(mol/m³)	Solubility C_L,/(mol/m³)	log K_{OW}	Henry's law constant H/(Pa·m³/mol) calculated P/C
Alkylphenols and other substituted phenols:							
Phenol	47	67.66	88360	938.9	1345	1.46	0.0500
o-Cresol (2-Methylphenol)		41	26000	240.4	237.32	1.98	0.1489
m-Cresol (3-Methylphenol)		16	22000	203.4	203.4	1.98	0.0786
p-Cresol (4-Methylphenol)		13	20000	184.9	230.6	1.96	0.0564
2,3-Dimethylphenol		8.05	6000	49.11	143.6		0.0560
2,4-Dimethylphenol		13.02	8795	71.99	71.99	2.35	0.1808
2,5-Dimethylphenol		10.68	3176	26.00	80.00		0.1335
2,6-Dimethylphenol		32.82	6230	51.00	81.60	2.36	0.4022
3,4-Dimethylphenol		2.241	5100	41.75	103.3	2.23	0.0217
3,5-Dimethylphenol		3.76	5500	45.02	107.2	2.35	0.0351
2,3,5-Trimethylphenol		2.43	800	5.874	28.24		0.0860
2,4,5-Trimethylphenol		7.73				2.67	
2,4,6-Trimethylphenol		19.58	1200	8.81	26.07	2.73	0.7511
3,4,5-Trimethylphenol		2.144	1540	11.31	73.91		0.0290
3-Methyl-5-ethylphenol		1.18	2314	16.99			
o-Ethylphenol		20.4	14042	114.9	114.9	2.47	0.1775
m-Ethylphenol		6.7				2.5	
p-Ethylphenol		5	7980	65.32	102.7	2.5	0.0487
2-Propylphenol		11.2				2.93	
4-Propylphenol		7.3	1728	12.69	12.69	3.2	0.5753
2-Isopropylphenol		12.45	4423	32.48	32.48	2.88	0.3834
4-Isopropylphenol			3263	23.96	55.59		
4-Butylphenol			617	4.107	4.107	3.65	
2-*sec*-Butylphenol		5				2.8	
2-*tert*-Butylphenol						2.7	
3-*tert*-Butylphenol			2070	13.78	20.38	2.6	
4-*sec*-Butylphenol		4	960	6.391	14.59	2.1	0.2741
4-*tert*-Butylphenol		1.24	580	3.861	20.11	3.04	0.0617
2-Methyl-5-*tert*-butylphenol		3.688	410	2.496			
2,6-Di-*sec*-butylphenol						4.4	

(Continued)

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TABLE 14.2.2 *(Continued)*

Compound	Selected properties: Vapor pressure P_S/Pa	Vapor pressure P_L/Pa	Solubility S/(g/m³)	Solubility C^S/(mol/m³)	Solubility $C_{L'}$/(mol/m³)	log K_{OW}	Henry's law constant H/(Pa·m³/mol) calculated P/C
3,5-Di-*tert*-butylphenol			14	0.0678	0.2816		
2,6-Di-*tert*-butyl-4-methylphenol		0.0338				4.17	
3-Pentylphenol						3.13	
4-Hexylphenol			391	2.193	2.568	3.6	
2-Heptylphenol						4.45	
4-Heptylphenol						4.15	
4-Octylphenol		0.071	12.6	0.0611	0.0917	4.12	0.7743
4-*tert*-Octylphenol						3.7	
2-Nonylphenol						5.76	
3-Nonylphenol						5.61	
4-Nonylphenol		0.1	5.43	0.0246	0.0362	4.48	2.764
1-Naphthol		0.5	438	3.038	14.75	2.84	0.0339
2-Naphthol		0.4	740	5.133	45.42	2.7	8.81×10^{B3}
2-Phenylphenol		30	700	4.113	8.568	3.09	3.501
4-Phenylphenol		8.7	9.8	0.0576	1.391	3.2	6.256
2-Allylphenol						2.64	
Chlorophenols:							
2-Chlorophenol	132	132	24650	191.7	191.7	2.17	0.6884
3-Chlorophenol	35	41.57	22000	171.1	203.2	2.5	0.2045
4-Chlorophenol	20	29.90	27000	210.0	313.9	2.4	0.0952
2,3-Dichlorophenol			8215	50.40	106.3	3.15	
2,4-Dichlorophenol	12	18.87	4500	27.61	43.41	3.2	0.4347
2,5-Dichlorophenol						3.2	
2,6-Dichlorophenol	12	32.09	2625	16.10	43.06	2.86	0.7451
3,4-Dichlorophenol			9256	56.79	149.8	3.37	
3,5-Dichlorophenol			7394	45.36	119.7	3.2	
2,3,4-Trichlorophenol	1	3.74	500	2.532	9.484	3.8	0.3949
2,3,5-Trichlorophenol	1	2.31	500	2.532	5.848	3.69	0.3949
2,3,6-Trichlorophenol			450	2.279	4.808	3.8	
2,4,5-Trichlorophenol	2.5	6.76	948	4.801	12.98	3.72	0.5207
2,4,6-Trichlorophenol	1.25	3.44	434	2.198	5.941	3.69	0.5687
3,4,5-Trichlorophenol						4.3	

(Continued)

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2,3,4,5-Tetrachlorophenol	0.1	0.79	166	0.7158	5.637	4.8	0.1397
2,3,4,6-Tetrachlorophenol	0.28	0.78	183	0.7892	2.180	4.45	0.3548
2,3,5,6-Tetrachlorophenol	0.1	0.78	100	0.4312	3.292	4.9	0.2319
Pentachlorophenol	4.15×10^{B3}	0.12	14	0.0526	1.524	5.05	0.0789
Nitrophenols:							
2-Nitrophenol		20	1080	7.764	12.15	1.8	1.646
3-Nitrophenol			11550	83.03	421.5	2	
4-Nitrophenol			13500	97.05	718.9	1.91	
2,4-Dinitrophenol			335	1.820	13.78	1.67	
2,4,6-Trinitrophenol (Picric acid)			13750	60.02	540.7	1.33	
4,6-Dinitro-*o*-cresol			222	1.120	4.500	2.12	
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:							
Catechol (1,2-Dihydroxybenzene)		1.34	45000	408.7	2462	0.88	5.44×10^{B4}
Resorcinol (1,3-Dihydroxybenzene)	0.0118	0.079	110000	999.0	6705	0.80	1.18×10^{B5}
Hydroquinone (1,4-Dihydroxybenzene)	2.55×10^{B3}	0.071	70000	635.7	17758	0.59	4.01×10^{B6}
2-Methoxyphenol (Guaiacol)	20.825	24.4	24800	199.8	233.9	1.33	0.1042
3-Methoxyphenol			67800	546.2	546.2	1.58	
4-Methoxyphenol			19500	157.1	323.9	1.34	
4-Chloroguaiacol			5370	33.86	33.86	2.15	
5-Chloroguaiacol			3960	24.97	30.94		
4,5-Dichloroguaiacol	0.570	1.72	575	2.98	9.000	3.26	0.1913
4,6-Dichloroguaiacol			708	3.668	8.754	2.86	
3,4,5-Trichloroguaiacol	0.163	0.64	310	1.363	5.344	3.77	0.1996
4,5,6-Trichloroguaiacol	0.032	0.23	54	0.2374	1.733	3.74	0.1348
Tetrachloroguaiacol	0.016	0.14	26	0.0993	0.8785	4.45	0.1612

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TABLE 14.2.3
Suggested half-life classes for phenolic compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Alkylphenols and other substituted phenols:				
Phenol	2	3	4	5
o-Cresol	1	2	3	4
p-Cresol	1	2	3	4
2,4-Dimethylphenol	2	3	4	5
Chlorophenols:				
2,4-Dichlorophenol	3	3	5	6
2,4,5-Trichlorophenol	4	4	6	7
2,4,6-Trichlorophenol	4	4	6	7
2,3,4,6-Tetrachlorophenol	5	5	6	7
Pentachlorophenol	5	5	6	7
Nitrophenols:				
2-Nitrophenol	3	3	5	6
4-Nitrophenol	3	3	5	6
2,4-Dinitrophenol	4	4	6	7
2,4,6-Trinitrophenol				
4,6-Dinitro-*o*-cresol	4	4	6	7
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:				
Catechol	2	3	4	5
2-Methoxyphenol (Guaiacol)	2	3	4	5
Tetrachloroguaiacol	4	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

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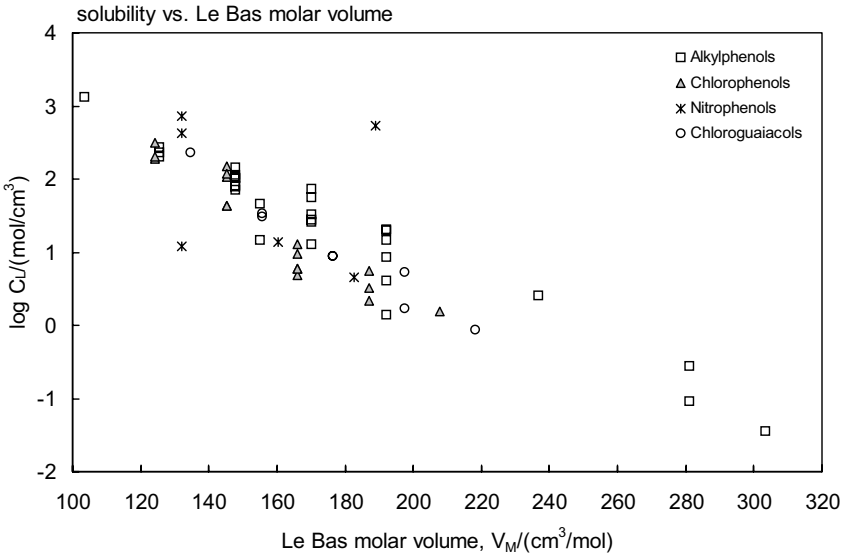

FIGURE 14.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

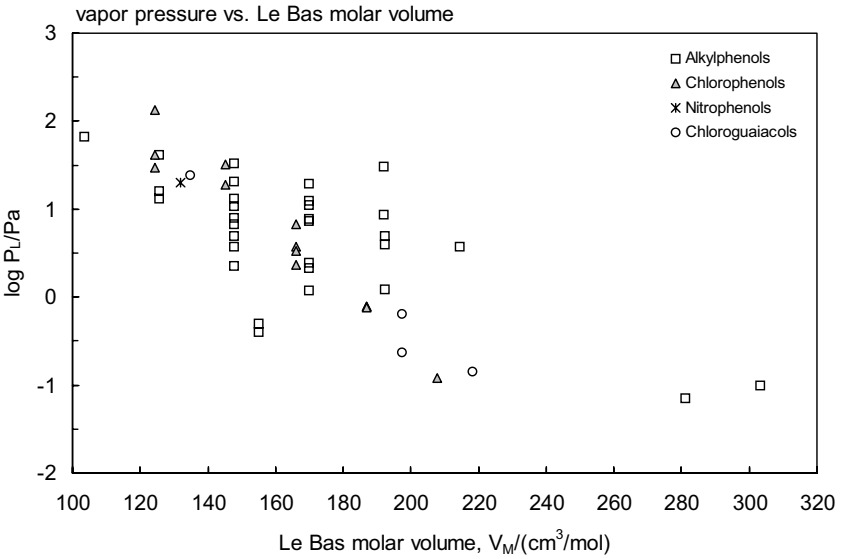

FIGURE 14.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

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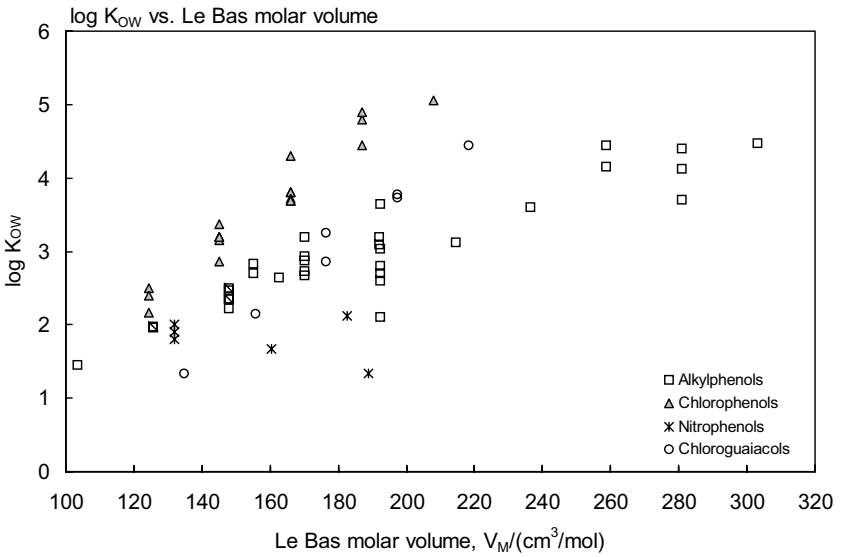

FIGURE 14.2.3 Octanol-water partition coefficient versus Le Bas molar volume for phenolic compounds.

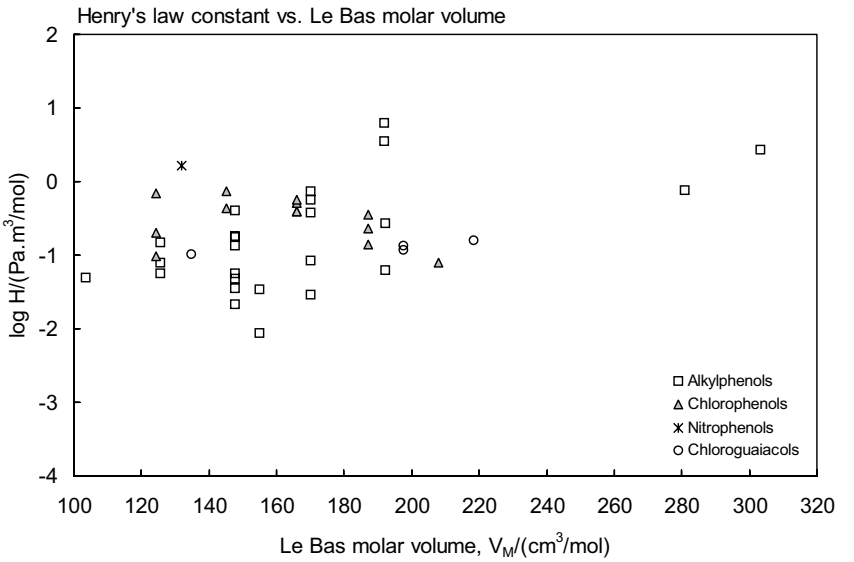

FIGURE 14.2.4 Henry's law constant versus Le Bas molar volume for phenolic compounds.

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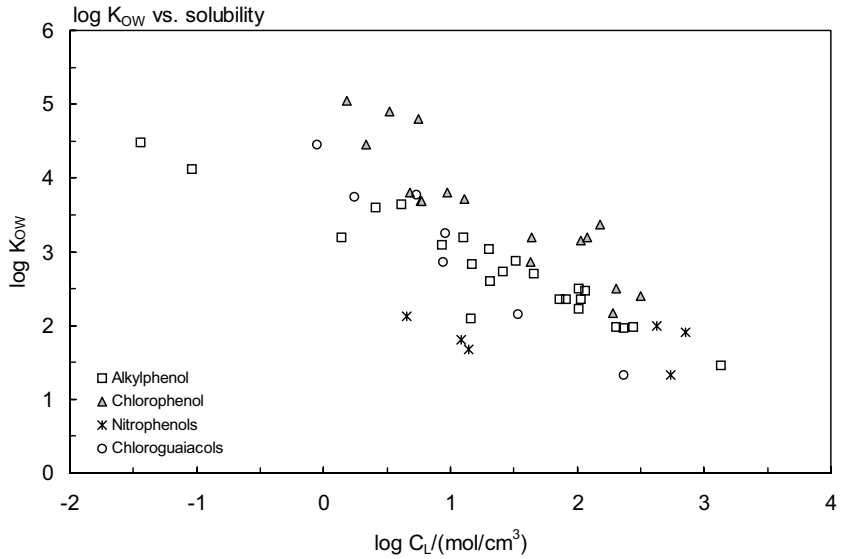

FIGURE 14.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for phenolic compounds.

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