11 Alcohols

CONTENTS

11.1 LIST OF CHEMICALS AND DATA COMPILATIONS

11.1.1 ALCOHOLS

11.1.1.1 Methanol

$$\begin{array}{c} H \\ | \\ H-\!\!\!-\!\!\!OH \\ | \\ H \end{array}$$
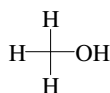
Common Name: Methanol
Synonym: methyl alcohol, carbinol, wood alcohol, wood spirit
CAS Registry No: 67-56-1
Molecular Formula: CH_3OH
Molecular Weight: 32.042
Melting Point (°C):
     –97.53   (Lide 2003)
Boiling Point (°C):
     64.6   (Lide 2003)
Density (g/cm³ at 20°C):
     0.7914   (Weast 1982–83)
Molar Volume (cm³/mol):
     42.5   (exptl. at normal bp, Lee et al. 1972; quoted, Reid et al. 1977)
     40.6   (calculated-density, Rohrschneider 1973)
     37.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

     miscible (Dean 1985; Howard 1990)

     miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
     temperatures designated * are compiled at the end of this section):
     16210*   (interpolated-regression of tabulated data, temp range –44.0 to 64.7°C, Stull 1947)
     16937*   (comparative ebulliometry, measured range 15–83.7°C, Ambrose & Sprake 1970)
     log (P/Pa) = 7.18411 – 1569.492/(T/K – 34.613); restricted temp range 15–39°C (Antoine eq., comparative
          ebulliometry, Ambrose & Sprake 1970)
     log (P/Pa) = 7.20519 – 1581.933/(T/K – 33.439); temp range 15–83.7°C (Antoine eq., comparative ebulliometry,
          Ambrose & Sprake 1970)
     16927   (vapor-liquid equilibrium VLE data, Polák & Lu 1972)
     log (P/mmHg) = [–0.2185 × 8978.8/(T/K)] + 8.639821; temp range –44 to 224°C (Antoine eq., Weast 1972–73)
     16958*   (static method, measured range 288.15–337.65 K, Gibbard & Creek 1974)
     12260, 21330   (20°C, 30°C, Verschueren 1983)
     16960   (calculated-Antoine eq., Boublik et al. 1984)
     log (P/kPa) = 7.24693 – 1806.615/(241.833 + t/°C); temp range 1.72–63.38°C (Antoine eq. from reported exptl.
          data, Boublik et al. 1984)
     log (P/kPa) = 7.20660 – 1582.698/(239.765 + t/°C); temp range 14–79.63°C (Antoine eq. from reported exptl.
          data of Ambrose & Sprake 1970, Boublik et al. 1984)
     log (P/kPa) = 7.023029 – 1595.671/(240.905 + t/°C), temp range 15–65°C (Antoine eq. derived from.exptl data
          of Gibbard & Creek 1974, Boublik et al. 1984)
     16670   (interpolated-Antoine eq., Dean 1985)
     log (P/mmHg) = 7.89750 – 1474.08/(229.13 + t/°C); temp range –14 to 65°C (Antoine eq., Dean 1985, 1992)
     log (P/mmHg) = 7.97328 – 1515.14/(232.85 + t/°C); temp range 64–110°C (Antoine eq., Dean 1985, 1992)
     16937   (Riddick et al. 1986)

log (P/kPa) = 7.20519 – 1581.993/(175.47 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 7.4182 – 1710.2/(–22.25 + T/K); temp range 175–273 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.25164 – 1608.39/(–31.07 + T/K); temp range 274–337 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.09489 – 1521.23/(–39.18 + T/K); temp range 338–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.86277 – 1105.884/(–64.272 + T/K); temp range 188–228 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.44355 – 1712.316/(–22.61 + T/K); temp range 224–290 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.26415 – 1615.59/(–30.437 + T/K); temp range 285–345 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.14736 – 1544.804/(–37.235 + T/K); temp range 335–376 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.27466 – 1641.542/(–25.789 + T/K); temp range 373–458 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)

log (P/mmHg) = 45.6171 – 3.2447 × 10^3/(T/K) –13.988·log(T/K) + 6.6365 × 10^{-3}·(T/K) – 1.0507 × 10^{-13}·(T/K)^2; temp range 175–513 K (vapor pressure eq., Yaws 1994)

35341   (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

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

0.446   (partial pressure-isoteniscope, Butler et al. 1935)
0.444   (entrainment method-GC, Burnett 1963)
0.472   (exptl., Hine & Mookerjee 1975)
0.367, 0.319   (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
0.45*   (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
0.451   (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
0.704   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
0.451   (limiting activity coefficient by headspace-GC., Li & Carr 1993)
0.620   (gas stripping-GC, Altschuh et al. 1999)
0.506   (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
ln K_{AW} = 8.969 – 5206.8/(T/K); temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
0.334   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 3.444 – 2142/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
1.239*   (40°C, headspace-GC, measured range 40–65°C, Teja et al. 2001)

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

–0.82   (shake flask-CR, Collander 1951)
–0.66   (shake flask-GC, Hansch & Anderson 1967)
–0.77 ± 0.02   (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
–0.52   (shake flask-RC, Cornford 1982)
–0.70   (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
–0.64, –0.63   (quoted, calculated-TSA, Iwase et al. 1985)
–0.71   (shake flask-GC at pH 7.0, Riebesehl & Tomlinson 1986)
–0.74   (recommended, Sangster 1989, 1993)
–0.77   (recommended value, Hansch et al. 1995)

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

2.98*   (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
2.84   (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

    4.45   (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)

    4.45   (alga *Chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)

    < 1.0   (golden ide, after 3 d, Freitag et al. 1985)

    4.46   (algae, after 1 d, Freitag et al. 1985)

    2.67   (activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

    –0.23   (calculated-MCI χ, Gerstl & Helling 1987)

    0.44   (soil, quoted exptl., Meylan et al. 1992)

    –0.36   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

    –1.08   (calculated-K_{OW}, Kollig 1993)

    0.44   (soil, calculated-MCI ^{1}χ, Sabljic et al. 1995)

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

Volatilization: $t_{1/2}$ ~ 5.3 h and 2.6 d for a model river 1-m deep and an environmental pond (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

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

$k_{OH} = (5.7 \pm 0.6) \times 10^8$ L mol^{-1} s^{-1} or 9.5×10^{-13} cm^3 molecule^{-1} s^{-1} at 292 K (relative rate method, Campbell et al. 1976)

$k_{OH} = (1.06 \pm 0.10) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k_{OH} = (1.00 \pm 0.10) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH} = 5.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 300 K (Lyman et al. 1982)

k ~ 0.024 M^{-1} s^{-1} for the reaction with O_3 in water at pH 2-5 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 0.76 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K in air (Meier et al. 1985; quoted, Atkinson 1985)

k_{OH}(calc) = 6.5×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 9.0×10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.80 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)

k_{OH}(exptl) = 0.90×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = 0.53×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH}* = $(8.61 \pm 0.47) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO3} < 6.0 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (flash photolysis-absorption technique (Wallington et al. 1987; selected, Atkinson 1991)

k(aq.) = 1.60×10^{-12} cm^3 molecule^{-1} s^{-1} for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

k_{OH}(exptl)* = 8.61×10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 240–440 (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 8.61 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}; k(soln) = 1.60×10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}* = 9.32×10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (9.0 \pm 0.9) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (1.0 \pm 0.23) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

k_{OH}(calc) = 4.05×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2} = 17.8$ d in ambient atmosphere (Howard 1990);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);

calculated lifetimes of 12 d and 1.0 yr for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.1.1
Reported vapor pressures of methanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(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)	
$\ln P = A - B/T/K) - C/(T/K)^2 + D/(T/K)^3$	(5)	

Stull 1947		Ambrose & Sprake 1970		Gibbard & Creek 1974			
summary of literature data		comparative ebulliometry		static method-manometer			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/kPa	T/K	P/kPa
–44.0	133.3	14.899	9815	288.1506	9.8844	323.1420	55.5900
–25.3	666.6	19.236	12468	288.1508	9.8858	323.1460	55.5996
–16.2	1333	23.323	15519	288.1511	9.8889	323.1490	55.5972
–6.0	2666	27.083	18858	288.1516	9.8867	328.1436	68.8187
5.0	5333	29.911	21769	293.1361	13.0023	328.1442	68.8158
12.1	7999	32.885	25206	293.1443	13.0119	328.1476	68.8450
21.2	13332	35.858	29128	293.1507	13.0109	328.1517	84.5907
34.8	26664	40.637	36493	293.1628	13.0228	333.1417	84.5859
49.9	53329	45.407	45347	298.1478	16.9558	333.1466	84.5940
64.7	101325	48.876	52883	298.1500	16.9562	333.1468	84.5859
		53.315	64036	298.1505	16.9578	333.1471	84.5940
mp/°C	–97.8	56.428	72975	298.1517	16.9584	337.6462	101.2523
		60.814	87345	303.1427	21.8743	337.6456	101.2526
		63.784	98330	303.1464	21.8782	337.6514	101.2742
		64.717	101998	303.1494	21.8823		
		68.403	117714	303.1503	21.8859	vapor pressure eq.	
		71.770	133741	308.1459	27.9763	eq. 5	P/kPa
		75.683	154640	308.1509	27.9844	A	15.6129944
		79.626	178306	308.1521	27.9871	10^3B	2.8459280
		83.678	205653	313.1500	35.4685	10^5C	3.743415457
				313.1504	35.4695	10^7D	2.188669628
		Antoine eq. for full range		313.1504	35.4714		
		eq. 3	P/Pa	313.1520	35.4654		
		A	7.20519	318.1475	44.5814		
		B	–1581.93	318.1477	44.5799		
		C	–33.439	318.1483	44.5829		
				318.1506	44.5833		
		data also fitted to Cragoe equation, eq. 5 see ref.					
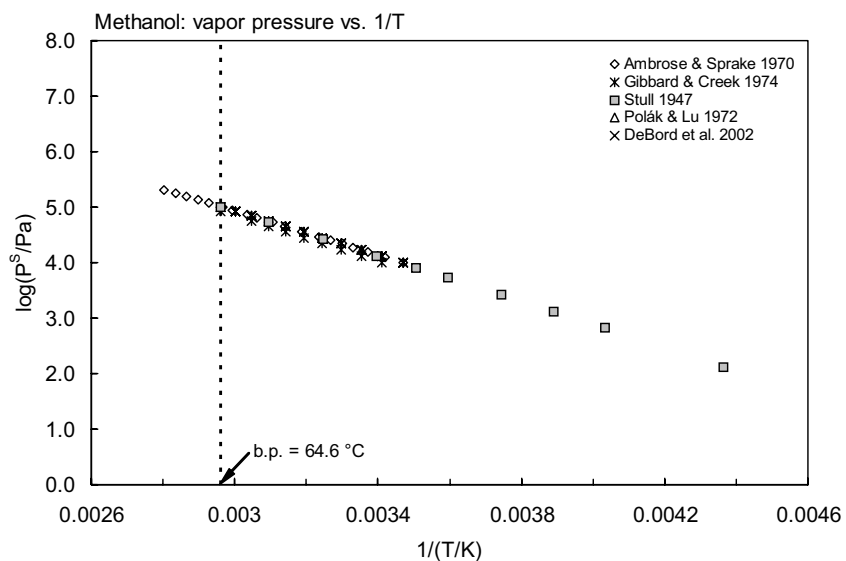
FIGURE 11.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanol.

TABLE 11.1.1.1.2
Reported Henry's law constants and octanol-air partition coefficients of methanol at various temperatures

Henry's law constant				log K_{OA}	
Snider & Dawson 1985		Teja et al. 2001		Gruber et al. 1997	
gas stripping-GC		headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
0	0.0908	40	1.239	20.29	2.98
25	0.4507	50	2.066	30.3	2.76
		60	3.656	40.4	2.56
enthalpy of transfer:		65	4.526	50.28	2.40
$\Delta H/(kJ\ mol^{-1}) = 41.0$					

Methanol: Henry's law constant vs. 1/T

FIGURE 11.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanol.

Methanol: K_{OA} vs. 1/T
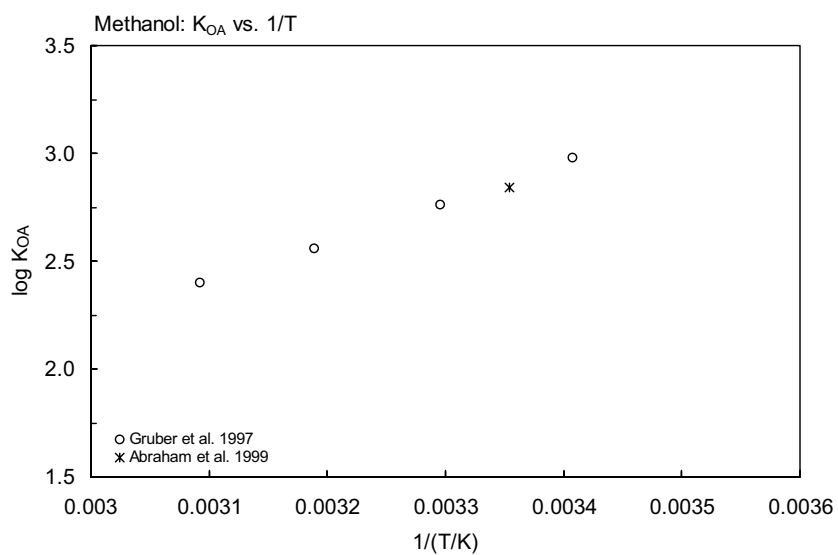

FIGURE 11.1.1.1.3 Logarithm of K_{OA} versus reciprocal temperature for methanol.

11.1.1.2   Ethanol

$\diagup\diagdown$OH

Common Name: Ethanol
Synonym: ethyl alcohol, methylcarbinol
Chemical Name: ethanol, ethyl alcohol
CAS Registry No: 64-17-5
Molecular Formula: CH_3CH_2OH
Molecular Weight: 46.068
Melting Point (°C):
    –114.14   (Lide 2003)
Boiling Point (°C):
    78.29   (Lide 2003)
Density (g/cm³ at 20°C):
    0.78933, 0.78505   (20°C, 25°C, Dreisbach & Martin 1949)
    0.7893   (Weast 1982–83)
Molar Volume (cm³/mol):
    58.6   (calculated-density, Rohrschneider 1973)
    59.2   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
    15.9   (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.02   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    miscible (Dean 1985)
    miscible (Riddick et al. 1986)
    miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    7314, 7581*   (24.4, 24.8°C, measured range 12.80–78.0°C, Kahlbaum 1883)
    6906*   (22.7°C, static method, measured range 22,7–78°C, Smyth & Engel 1929)
    7599   (gas saturation/air-bubbling method, Washburn & Handorf 1935)
    39345*   (vapor-liquid equilibrium VLE data, measured range 35–60°C, Scatchard & Raymond 1938)
    7538*   (interpolated-regression tabulated data, temp range –31.3 to 78.4°C, Stull 1947)
    1593, 7869, 29456   (0, 25, 50°C, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)
    7869*   (static method, measured range 0–78.553°C, Kretschmer & Wiebe 1949)
    log (P/mmHg) = 8.11576 – 1595.76/(t/°C + 226.5); temp range 0–78.553°C, Kretschmer & Wiebe 1949)
    log (P/mmHg) = 8.24169 – 1652.6/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    7870*   (comparative ebulliometry, measured range 19.622–93.5°C, Ambrose & Sprake 1970)
    log (P/Pa) = 7.16879 – 1552.601/(T/K – 50.731); restricted temp range 19.6–43.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
    log (P/Pa) = 7.24739 – 1599.039/(T/K – 46.391); temp range 19.6–93.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
    7865   (vapor-liquid equilibrium VLE data, Polák & Lu 1972)
    log (P/mmHg) = [–0.2185 × 9673.6/(T/K)] + 8.827392; temp range –31.3–242°C (Antoine eq., Weast 1972–73)
    5852, 6665, 9998   (20, 25, 30°C, Verschueren 1983)
    8060   (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 7.24222 – 1595.811/(226.448 + t/°C); temp range 19.62–93.48°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 4.11678 – 323.237/(74.916 + t/°C); temp range 12.8–78.2°C (Antoine eq. from reported exptl. data of Kahlbaum 1883, Boublik et al. 1984)

log (P/kPa) = 7.31243 – 1630.868/(229.581 + t/°C); temp range 0–78.55°C (Antoine eq. from reported exptl. data of Kretschmer & Wiebe 1949, Boublik et al. 1984)

7968   (calculated-Antoine eq., Dean 1985)

log (P/mmHg) = 8.32109 – 1718.10/(237.52 + t/°C); temp range –2 to 100°C (Antoine eq., Dean 1985, 1992)

7870   (Riddick et al. 1986)

log (P/kPa) = 7.16879 – 1552.601/(222.419 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 7.15946 – 1547.464/(–51.177 + T/K); temp range 320–359 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.23347 – 1591.28/(–47.056 + T/K), temp range: 292–367 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.9391 – 2381.5/(T/K); temp range 210–271 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.5224 – 2299/(T/K); temp range 193–223 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.16386 – 1550.006/(–50.941 + T/K); temp range 320–359 K, (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.27664 – 1615.127/(–45.012 + T/K); temp range 292–353 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.95131 – 1423.668/(–63.568 + T/K); temp range 349–374 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

log (P/mmHg) = 23.8442 – 2.8642 × 10^3/(T/K) –5.0474·log(T/K) + 3.7448 × 10^{-11}·(T/K) + 2.7361 × 10^{-5}·(T/K)^2; temp range 159–516 K (vapor pressure eq., Yaws 1994)

17819   (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

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

0.520   (partial pressure-isoteniscope, Butler et al. 1935)
0.0118   (partial vapor pressure, concn.-GC, Burnett & Swoboda 1962)
0.4660   (entrainment method-GC, Burnett 1963)
0.637   (exptl.-calculated C_W/C_A, Hine & Mookerjee 1975)
0.495, 0.472   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.527*   (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
0.530   (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
0.637   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
0.823   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
0.70   (correlated-molecular structure, Russell et al. 1992)
0.542   (limiting activity coefficient by headspace-GC., Li & Carr 1993)
0.593   (solid-phase microextraction SPME-GC, Bartelt 1997)
0.744   (gas stripping-GC, Altschuh et al. 1999)
0.568   (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
ln K_{AW} = 10.173 – 5531.6/(T/K); temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
0.361   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 5.576 – 2757/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

–0.32   (shake flask-CR, Collander 1951)
–0.16   (Leo et al. 1969; Hansch & Dunn III 1972)
–0.30   (shake flask-GC, Dillingham et al. 1973)
–0.31 ± 0.02   (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
–0.22, –0.20   (calculated-f const., Rekker 1977)
–0.18   (shake flask-RC, Cornford 1982)

–0.20   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
–0.30   (recommended, Sangster 1989, 1993)
–0.25   (thermometric titration, Fujiwara et al. 1991)
–0.29   (calculated-activity coeff. γ from UNIFAC, Dallos et al. 1993)
–0.31, –0.22   (recommended value; value at pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated
   * are compiled at the end of this section:
   3.34*   (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber
         et al. 1997)
   3.20   (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
   –1.63   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:
   0.09   (calculated- MCI χ, Gerstl & Helling 1987)
   0.20   (soil, exptl., Meylan et al. 1992)
   –0.14   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
   0.20   (soil, calculated-MCI ^{1}χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
   Volatilization: $t_{1/2}$ ~ 6 d from water (estimated, Howard 1990).
   Photolysis:
   Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
      with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression
      see reference:
      k = 0.01 M^{-1} s^{-1} for oxidation by RO$_2$ radical at 30°C in aquatic systems with $t_{1/2}$ = 8 × 10^5 d (Howard 1972;
         Hendry et al. 1974; quoted, Mill 1982)
      photooxidation $t_{1/2}$ = 0.24–2.4 h based on the rate of disappearance of hydrocarbon due to reaction with OH
         radical (Darnall et al. 1976)
      k_{OH} = (1.8 ± 0.2) × 10^9 L mol^{-1} s^{-1} or 3.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 292 K (relative rate method, Campbell
         et al. 1976)
      k = < 2 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen in aquatic systems at 25°C with $t_{1/2}$ > 100 yr (Foote
         1976; Mill 1979; Mill 1982)
      k_{OH} = 2 × 10^9 L mol^{-1} s^{-1} at 25°C in the atmosphere with $t_{1/2}$ = 2.8 d (Hendry & Kenley 1979)
      k_{OH} = (3.74 ± 0.37) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (Overend & Paraskevopoulos 1978)
      k_{OH} = 1.8 × 10^{12} cm^3 mol^{-1} s^{-1} at 300 K (Lyman et al. 1982)
      k_{OH} = (2.62 ± 0.36) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Ravishan-
         kara & Davis 1978)
      k_{OH} = 1.75 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Meier et al. 1985)
      k(aq.) = (0.37 ± 0.04) M^{-1} s^{-1} for the reaction with O$_3$ in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
      k_{OH} = 2.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)
      k_{OH}(calc) = 3.3 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR
         structure-activity relationship, Atkinson 1987)
      k_{OH}(exptl) = 2.9 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = 3.1 × 10^{-12} cm^3·molecule^{-1} s^{-1} at room temp. (SAR
         structure-activity relationship, Atkinson 1987)
      k_{OH}* = (33.3 ± 2.3) × 10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 240–440 K (flash photolysis-
         resonance fluorescence, Wallington & Kurylo 1987a)
      k_{NO3} < 9.0 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al.
         1987; quoted, Atkinson 1991)
      k_{OH}* = 3.33 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance
         fluorescence, Wallington et al. 1988a)
      k_{OH} = 3.33 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k(soln) = 3.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} for the solution-phase reaction
         with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}* = 3.27×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k_{OH} = $(3.04 \pm 0.25) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = $(3.46 \pm 0.52) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

k(aq.) = 0.51 M^{-1} s^{-1} at pH 7.2, k = 0.72 M^{-1} s^{-1} at pH 7.3, and k = 0.77 M^{-1} s^{-1} at pH 8.1 for direct reaction with ozone in water at 21°C with $t_{1/2}$ = 18 h at pH 7 (Yao & Haag 1991)

k_{OH}(calc) = 5.16×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$t_{1/2}$(aq. aerobic) = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Malaney & Gerhold 1969; selected, Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

k = 0.0043–0.055 h^{-1} in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

$t_{1/2}$ ~ 5.9 d to 4.0 d estimated in the atmosphere (Graedel 1978; quoted, Howard 1990), based on the reaction with a OH radical concentration of 8×10^5 molecules/cm^3 (Campbell 1976; Lyman et al. 1982; quoted, Howard 1990);

photooxidation $t_{1/2}$ = 12.2–122 h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);

calculated lifetimes of 3.5 d and 26 d for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000).

Surface water: photooxidation $t_{1/2}$ = 334 d -36.6 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; selected, Howard et al. 1991); measured rate constants of 0.51 M^{-1} s^{-1}, 0.72 M^{-1} s^{-1}, 0.77 M^{-1} s^{-1}, at pH 7.2, 7.3, 8.1, respectively, for direct reaction with ozone in water at 21°C, with $t_{1/2}$ = 18 h at pH 7 (Yao & Haag 1991).

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

Sediment:

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

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TABLE 11.1.1.2.1

Reported vapor pressures of ethanol 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)		

Kahlbaum 1883		Scatchard & Raymond 1938		Kretschmer & Wiebe 1949		Ambrose & Sprake 1970	
Ber. 16, 2476 (1883)		vapor-liquid equilibrium		static method, VLE data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.80	2733	35	13703	0.0	1593	19.622	5726
17.4	4114	40	17877	25.0	7869	23.633	7269
21.0	5509	45	23033	34.988	13736	25.722	8205
24.4	7314	50	29488	44.994	23058	28.157	9430
24.8	7581	55	37312	50.0	29456	33.334	12566

(Continued)

TABLE 11.1.1.2.1 (*Continued*)

Kahlbaum 1883		Scatchard & Raymond 1938		Kretschmer & Wiebe 1949		Ambrose & Sprake 1970	
Ber. 16, 2476 (1883)		vapor-liquid equilibrium		static method, VLE data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
26.2	8261	60	46839	54.988	37302	36.606	14981
78.0	101325	65	58443	65.0	58400	39.237	17200
		70	72273	78.553	102219	43.228	21109
		85	88858			47.349	25914
				eq. 2	P/mmHg	51.081	31047
				A	8.11576	54.554	36760
Smyth & Engel 1929		**Stull 1947**		B	1595.76	58.873	44584
static-manometry		summary of literature data		C	226.5	62.865	53267
t/°C	P/Pa	t/°C	P/Pa			66.578	62572
						70.559	74032
22.7	6906	–31.3	133.3			74.980	88763
32.6	12012	–12.0	666.6			77.485	97821
35.7	14079	–2.30	1333			77.989	100121
41.8	19345	8.0	2666			78.340	101518
57.2	40903	19.0	5333			78.497	102151
59.6	45690	26.0	7999			79.188	104983
69.4	70808	34.9	13332			82.363	118791
78.1	99672	48.4	26664			85.836	135519
78.4	101325	63.5	53329			89.606	155824
		78.4	101325			93.481	179321
bp/°C	78.4–78.5						
		mp/°C	–112				

FIGURE 11.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethanol.

TABLE 11.1.1.2.2
Reported Henry's law constants and octanol-water partition coefficients of ethanol at various temperatures

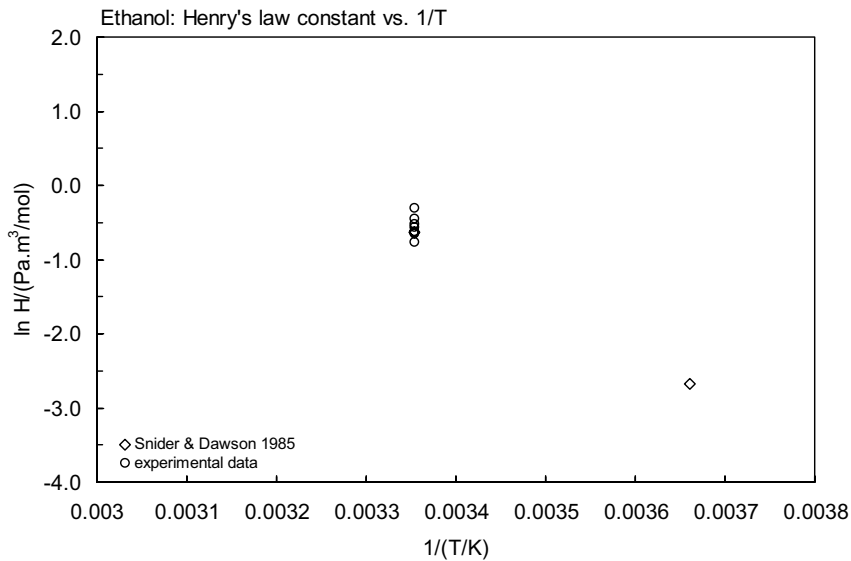| Henry's law constant		log K_{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
0	0.0688	20.29	3.34
25	0.5274	30.3	3.10
		40.4	2.87
enthalpy of transfer:		50.28	2.69
$\Delta H/(kJ\ mol^{-1}) = 54.392$			

FIGURE 11.1.1.2.2 Logarithm of Henry's law constant versus reciprocal temperature for ethanol.
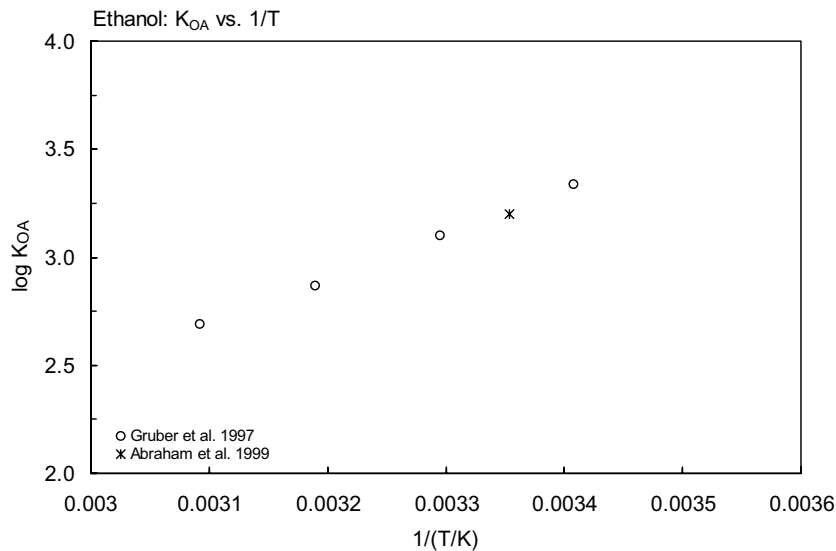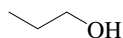

FIGURE 11.1.1.2.3 Logarithm of K_{OA} versus reciprocal temperature for ethanol.

11.1.1.3 Propanol (*n*-Propyl alcohol)

Common Name: Propanol
Synonym: propyl alcohol, 1-propanol, *n*-propyl alcohol
Chemical Name: propanol, propyl alcohol, *n*-propyl alcohol
CAS Registry No: 71-23-8
Molecular Formula: C_3H_8O, $CH_3CH_2CH_2OH$
Molecular Weight: 60.095
Melting Point (°C):
    –124.39   (Lide 2003)
Boiling Point (°C):
    97.2   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8035   (Weast 1982–83)
    0.8037   (Dean 1985)
Molar Volume (cm³/mol):
    75.1   (calculated-density, Rohrschneider 1973)
    81.4   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK:
    19.4   (pK$_s$, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.372   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    > 3.1×10^6 (Booth & Everson 1948)
    miscible (Dean 1985; Riddick et al. 1986, Yaws et al. 1990))

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    2844   (saturated vapor density-gas saturation, Puck & Wise 1946)
    2594*   (interpolated-regression of tabulated data, temp range –15 to 97.8°C, Stull 1947)
    10990*   (48.14°C, measured range 48.14–97.1°C, Brown & Smith 1959)
    2720*   (ebulliometry-differential thermal analysis, measured range 19.3–97.3°C, Kemme & Kreps 1969)
    log (P/mmHg) = 8.18894 – 1690.864/(221.346 + t/°C); temp range 19.3–97.3°C, or pressure range 14.7–758.5
        mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
    2798*   (comparative ebulliometry, measured range 60.2–104.5°C, Ambrose & Sprake 1970)
    log (P/Pa) = 6.74390 – 1365.579/(T/K – 82.093); restricted temp range 60.2–81.2°C (Antoine eq., comparative
        ebulliometry, Ambrose & Sprake 1970)
    log (P/Pa) = 6.87613 – 1441.705/(T/K – 74.291); temp range 60.2–104.5°C (Antoine eq., comparative ebulliom-
        etry, Ambrose & Sprake 1970)
    log (P/mmHg) = [–0.2185 × 10421.1/(T/K)] + 8.937293; temp range –15 to 250°C (Antoine eq., Weast 1972–73)
    2744   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.97878 – 1497.734/(204.094 + t/°C); temp range 48.14–94.36°C (Antoine eq. from reported exptl.
        data of Brown & Smith 1959, Boublik et al. 1984)
    log (P/kPa) = 6.87065 – 1438.587/(198.552 + t/°C); temp range 60.2–104.6°C (Antoine eq. from reported exptl.
        data of Ambrose & Sprake 1970, Boublik et al. 1984)
    2780   (interpolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 7.84767 – 1499.21/(204.64 + t/°C); temp range 2–120°C (Antoine eq., Dean 1985, 1992)
    2798   (Riddick et al. 1986)
    log (P/kPa) = 6.87613 – 1441.705/(198.859 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log $(P_L/\text{kPa}) = 6.86874 – 1437.906/(–74.621 + T/K)$; temp range 333–378 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 6.74195 – 1364.911/(–82.114 + T/K)$; temp range 356–378 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 8.7592 – 2506/(T/K)$; temp range 200–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 6.74403 – 1366.08/(–81.994 + T/K)$; temp range 356–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 6.87377 – 1440.743/(–74.344 + T/K)$; temp range 333–376 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 6.58415 – 1273.365/(–92.178 + T/K)$; temp range 369–407 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log $(P/\text{mmHg}) = 31.5155 – 3.457 \times 10^3/(T/K) – 7.5235 \cdot \log (T/K) – 4.287 \times 10^{-11} \cdot (T/K) + 1.3029 \times 10^{-7} \cdot (T/K)^2$; temp range 124–537 K (vapor pressure eq., Yaws 1994)

6939   (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

9470   (45.43°C, vapor-liquid equilibrium VLE data, measured range 45.43–58.9°C, Pasanen et al. 2004)

5876   (37.02°C, ebulliometric method, measured range 310.17–356.7 K, Lubomska & Malanowski 2004)

log $(P/\text{kPa}) = 7.219284 – 1629.492/[(T/K) – 57.556]$; temp range 310.17–356.7 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

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

0.694   (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

0.620   (entrainment method-GC, Burnett 1963)

0.683   (exptl., Hine & Mookerjee 1975)

0.699; 0.710   (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

0.751*   (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

0.683   (limiting activity coefficient by headspace-GC., Abraham et al. 1987)

0.925   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

0.683, 0.942   (quoted, correlated-molecular structure, Russell et al. 1992)

0.715   (limiting activity coefficient by headspace-GC., Li & Carr 1993)

1.034   (solid-phase microextraction SPME-GC, Bartelt 1997)

0.372   (wetted-wall column-GC, Altschuh et al. 1999)

0.802   (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

ln $K_{AW} = 11.830 – 5923.2/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

0.490   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log $K_{AW} = 6.955 – 3123/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.34   (shake flask-GC, Hansch & Anderson 1967)

0.30   (shake flask-GC, Dillingham et al. 1973)

0.25 ± 0.01 (shake flask-GC, Leo et al. 1975)

0.29   (Hansch & Leo 1979)

0.32   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)

0.25   (recommended, Sangster 1989)

0.25   (recommended value, Hansch et al. 1995)

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

3.85*   (20.29°C, from GC determined $\gamma°$ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

–1.069   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

    0.37   (calculated-MCI χ, Gerstl & Helling 1987)
    0.48   (soil, quoted exptl., Meylan et al. 1992)
    0.12   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
    0.48   (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

    Volatilization:

    Photolysis:

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

        photooxidation $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

        k_{OH} = (2.3 ± 0.2) × 10^9 L mol^{-1} s^{-1} at 292 K (relative rate method, Campbell et al. 1976)

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

        k_{OH} = 2 × 10^9 M^{-1} s^{-1} at 25°C with $t_{1/2}$ = 2.8 d (Hendry & Kenley 1979; quoted, Mill 1982)

        k_{OH} = (5.33 ± 0.53) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

        k = (0.37 ± 0.04) M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

        k_{OH}(calc) = 5.3 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 5.3 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

        k_{OH}(exptl) = 5.3 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 5.0 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

        k_{OH} = (5.34 ± 0.29) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

        k_{OH} = 5.34 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 4.7 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)

        k_{OH}* = 5.34 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} 298 K (recommended, Atkinson 1989, 1990)

        k_{OH} = (5.64 ± 0.48) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = (5.50 ± 0.44) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

        k_{OH}(calc) = 6.8 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1996)

    Hydrolysis:

    Biodegradation: average rate of biodegradation 71.0 mg COD g^{-1} h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

    Biotransformation:

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

Half-Lives in the Environment:

    Air: $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

    Surface water:

    Groundwater:

    Sediment:

    Soil:

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TABLE 11.1.1.3.1
Reported vapor pressures of propanol 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)		

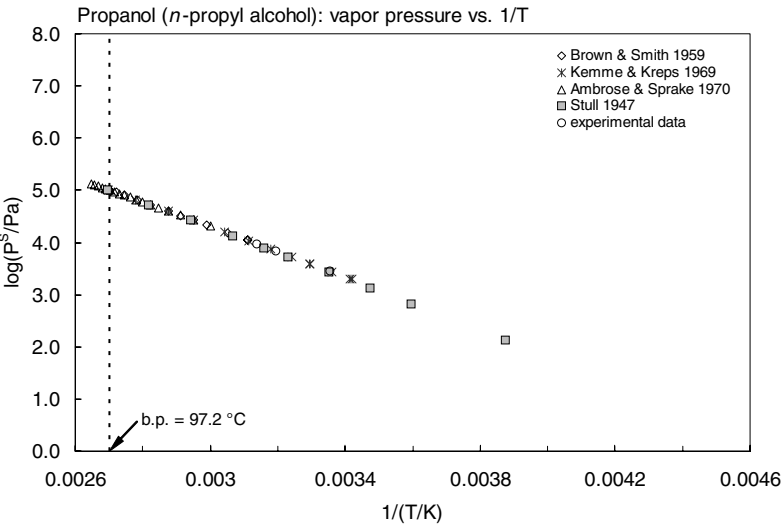| Stull 1947		Brown & Smith 1959		Kemme & Kreps 1969		Ambrose & Sprake 1970	
summary of literature data				differential thermal analysis		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				ebulliometry			
–15.0	133.1	48.14	10990	19.3	1960	60.168	20438
5.0	666.6	48.16	10996	19.8	1987	65.599	26579
14.7	1333	48.18	11018	24.5	2720	70.255	33024
25.3	2666	54.52	15405	30.3	3920	74.507	40001
36.4	5333	61.51	21851	30.3	3933	78.022	46676
43.5	7999	65.80	26867	35.2	5293	81.174	53435
52.8	13332	70.09	32831	41.3	7519	83.931	59974
66.8	26664	74.56	40177	48.1	10839	86.490	66638
82.0	53329	81.11	53379	55.4	16052	88.856	73334
97.8	101325	97.08	101358	65.7	26584	91.026	79952
		97.09	101331	74.6	39997	93.143	86877
mp/°C	–127	97.10	101393	86.6	66461	94.955	93192
		86.0	65456	97.3	101125	96.837	100132
		91.13	80472			97.595	103031
		94.36	91342	Antoine eq.		98.513	106666
				eq. 2	P/mmHg	100.155	113408
				A	8.18894	101.666	119903
				B	1690.864	103.166	126648
				C	221.346	104.515	133259
				$\Delta H_V/(kJ\ mol^{-1})$			
				at bp	56.066		

FIGURE 11.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propanol.

TABLE 11.1.1.3.2
Reported Henry's law constants and octanol-air partition coefficients of propanol at various temperatures

Henry's law constant		log K_{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
0	0.0757	20.29	3.85
25	0.7512	30.3	3.56
		40.4	3.33
enthalpy of transfer:		50.28	3.11
$\Delta H/(kJ\ mol^{-1}) = 58.576$			

Propanol (*n*-propyl alcohol): Henry's law constant vs. 1/T
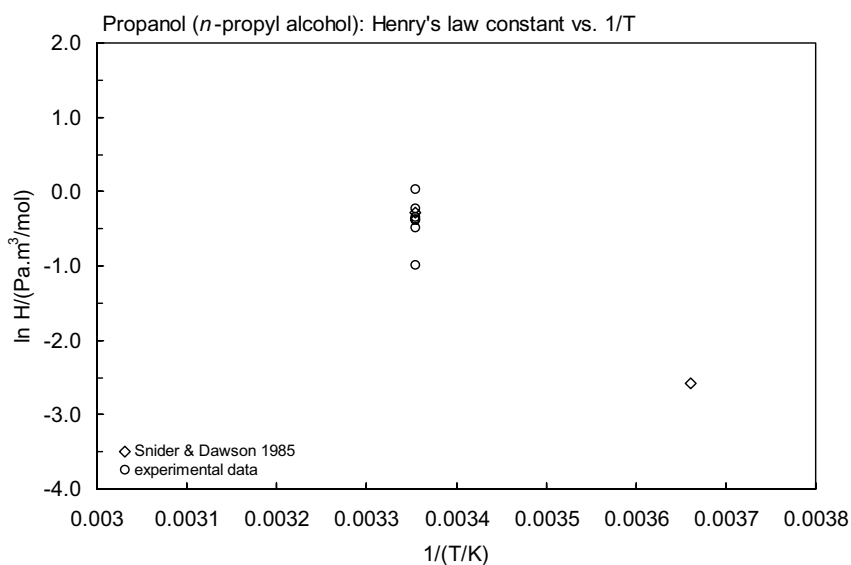
FIGURE 11.1.1.3.2 Logarithm of Henry's law constant versus reciprocal temperature for propanol.

Propanol (*n*-propyl alcohol): K_{OA} vs. 1/T
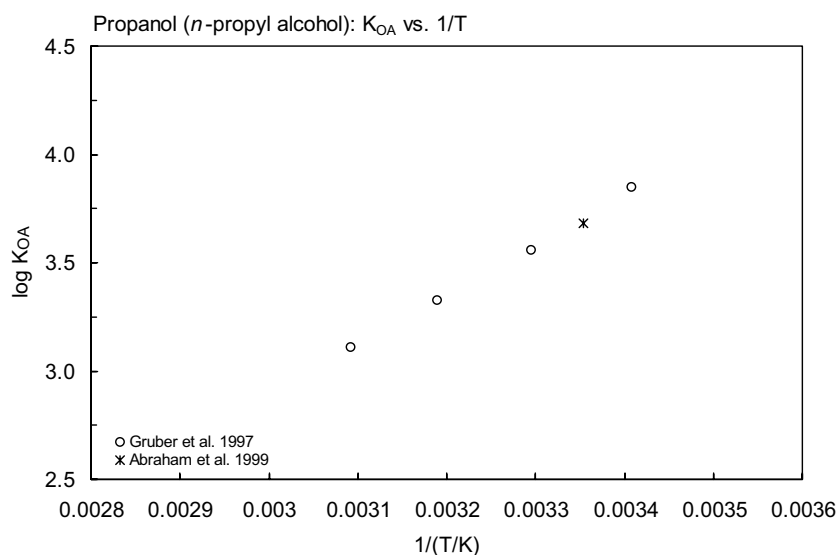
FIGURE 11.1.1.3.3 Logarithm of K_{OA} versus reciprocal temperature for propanol.

11.1.1.4 Isopropanol (*i*-Propyl alcohol)

Common Name: Isopropanol
Synonym: isopropyl alcohol, 2-propanol, *i*-propyl alcohol, dimethylcarbinol, *sec*-propylalcohol, perspirit, petrohol, avantine, IPA
Chemical Name: isopropanol, isopropyl alcohol, *i*-propyl alcohol
CAS Registry No: 67-63-0
Molecular Formula: C_3H_8O, $CH_3(CH_3)CHOH$
Molecular Weight: 60.095
Melting Point (°C):
    –87.9   (Lide 2003)
Boiling Point (°C):
    82.3   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7812   (25°C, Butler et al. 1935)
    0.7855   (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
    76.8   (calculated-density, Rohrschneider 1973)
    81.4   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
    17.1   (Serjeant & Dempsey 1979; Howard 1990)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.406   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    > 3.1×10^6 (Booth & Everson 1948)
    miscible (Dean 1985; Riddick et al. 1986; Howard 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    5866*   (static method-isoteniscope, measured 0–90°C, Parks & Barton 1928)
    5700*   (interpolated-regression of tabulated data, temp range –26.1 to 82.5°C, Stull 1947)
    5775*   (comparative ebulliometry, measured range 52.323–89.261°C, Ambrose & Sprake 1970)
    $\log (P/Pa) = 6.73896 – 1290.345/(T/K – 82.778)$; restricted temp range 52.3–71.1°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
    $\log (P/Pa) = 6.86618 – 1360.131/(T/K – 75.558)$; temp range 52.3–89.3°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
    $\log (P/mmHg) = [–0.2185 \times 10063.5/(T/K)] + 7.805751$; temp range –91 to 160°C (Antoine eq., Weast 1972–73)
    4266, 7588 (20°C, 30°C, Verschueren 1983)
    5070; 5700 (extrapolated-Antoine eq., Boublik et al. 1984)
    $\log (P/kPa) = 6.86634 – 1360.183/(197.593 + t/°C)$; temp range 52.3–89.26°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
    $\log (P/kPa) = 6.358 – 1082.462/(166.482 + t/°C)$; temp range 81.61–147.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    6021   (calculated-Antoine eq., Dean 1985)
    $\log (P/mmHg) = 8.11778 – 1580.92/(219.61 + t/°C)$; temp range 0–101°C (Antoine eq., Dean 1985, 1992)
    5775   (Riddick et al. 1986)
    $\log (P/kPa) = 6.86618 – 1360.131/(126.36 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

log $(P_L/kPa) = 6.86087 – 1357.514/(–75.786 + T/K)$; temp range 325–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.72348 – 1282.26/(–83.591 + T/K)$; temp range 347–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 9.681 – 2626/(T/K)$; temp range 195–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.73782 – 1290.039/(–82.771 + T/K)$; temp range 347–363 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.86451 – 1359.473/(–75.592 + T/K)$; temp range 325–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.61939 – 1225.439/(–89.774 + T/K)$; temp range 350–383 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log $(P/mmHg) = 38.2363 – 3.5513 \times 10^3/(T/K) – 10.031 \cdot \log(T/K) – 3.474 \times 10^{-10} \cdot (T/K) + 1.7367 \times 10^{-6} \cdot (T/K)^2$; temp range 185–508 K (vapor pressure eq., Yaws 1994)

13806   (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

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

0.814   (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

0.820   (exptl., Hine & Mookerjee 1975)

1.159, 0.710   (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)

0.80*   (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

1.131   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

3.16*   (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

ln $(1/K_{AW}) = –10.6 + 5413/(T/K)$; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

0.820, 0.715 (quoted, correlated-molecular structure, Russell et al. 1992)

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

5.55   (EPICS-GC, Ayuttaya et al. 2001)

0.521   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log $K_{AW} = 5.576 – 2757/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

2.186 – 0.666   (27°C, equilibrium headspace-GC, solute concn 12.31-125.08 mg/L, measured range 300–315 K, Cheng et al. 2003)

2.186*   (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

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

0.14   (Leo et al. 1969; Hansch & Dunn III 1972)

0.05   (shake flask-GC, Dillingham et al. 1973)

0.05   (Hansch & Leo 1985)

0.14   (HPLC-k' correlation, Funasaki et al. 1986)

0.55   (UNIFAC activity coefficient, Banerjee & Howard 1988)

0.05   (recommended, Sangster 1989, 1993)

0.05   (recommended, Hansch et al. 1995)

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

3.54*   (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization: the estimated $t_{1/2}$ ~3.6 d for evaporation from water 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

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

photooxidation $t_{1/2}$ = 197 d to 22 yr in water, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

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

k_{OH} = 4.1×10^9 M^{-1} s^{-1} at 25°C with $t_{1/2}$ = 1.3 d (Hendry & Kenley 1979; quoted, Mill 1982)

k_{OH} = $(5.48 \pm 0.55) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at (296 ± 2) K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

k_{OH} = 4.3×10^{12} cm^3 mol^{-1} s^{-1} at 300 K (Lyman et al. 1982)

k = (1.9 ± 0.2) M^{-1} s^{-1} for the reaction with ozone in water at pH 2-6 and 20–23°C (Hoigné & Bader 1983)

k_{OH}(calc) = 7.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 6.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

k_{OH}(exptl) = 6.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and k_{OH}(calc) = 6.6×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH}* = $(5.81 \pm 0.34) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

k_{NO3} < 2.3×10^{-15} cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)

k(aq.) = 3.20×10^{-12} cm^3 $molecule^{-1}\cdot s^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

k_{OH}(exptl)* = 5.81×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

k_{OH} = 5.81×10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 3.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}* = 5.21×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k_{OH} = $(5.69 \pm 1.09) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = $(5.78 \pm 0.753) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

k_{OH}(calc) = 2.90×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

k = 52.0 mg COD g^{-1} h^{-1}, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$ (aq. aerobic) = 24–168 h, based on unacclimated aerobic aqueous screening test data (Gellman & Heukelekian 1955; Heukelekian & Rand 1955; Price et al. 1974; Takemoto et al. 1981; Wagner 1976; selected, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 96–672 h, based on estimated aerobic aqueous biodegradation half-life and unacclimated anaerobic aqueous screening test data (Hou et al. 1983; Sonoda & Seiko 1968; Speece 1983; selected, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2}$ = 6.2–72 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985, 1987; quoted, Howard 1990; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2}$ = 197 d to 22 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2}$ = 26–168 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

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

Sediment:

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

Biota:

TABLE 11.1.1.4.1
Reported vapor pressures of isopropanol 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)	

Parks & Barton 1928		Stull 1947		Ambrose & Sprake 1970	
static method/isoteniscope		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	1187	–26.1	133.1	52.323	26540
5	1613	–7.00	666.6	56.779	33044
10	2266	2.40	1333	60.798	40017
15	3173	12.7	2666	64.091	46612
20	4320	23.8	5333	67.087	53371
25	5866	30.5	7999	69.704	59931
30	7879	39.5	13332	72.131	66601
35	10519	53.0	26664	74.372	73286
40	14079	67.8	53329	76.454	79997
45	18239	82.5	101325	78.431	86822
50	23571			80.160	93175
55	30318	mp/°C	–85.8	81.931	100078
60	38464			82.958	104266
65	48409			85.090	113416
70	60635			86.550	120046
75	74847			87.992	126573
80	92232			89.261	133218
85	112737				
90	136082				

$\Delta H_V/(kJ\ mol^{-1})$ =
  at 25°C   44.43
    at bp   40.166

Isopropanol (*i*-propyl alcohol): vapor pressure vs. 1/T

◇ Parks & Barton 1928
△ Ambrose & Sprake 1970
▢ Stull 1947
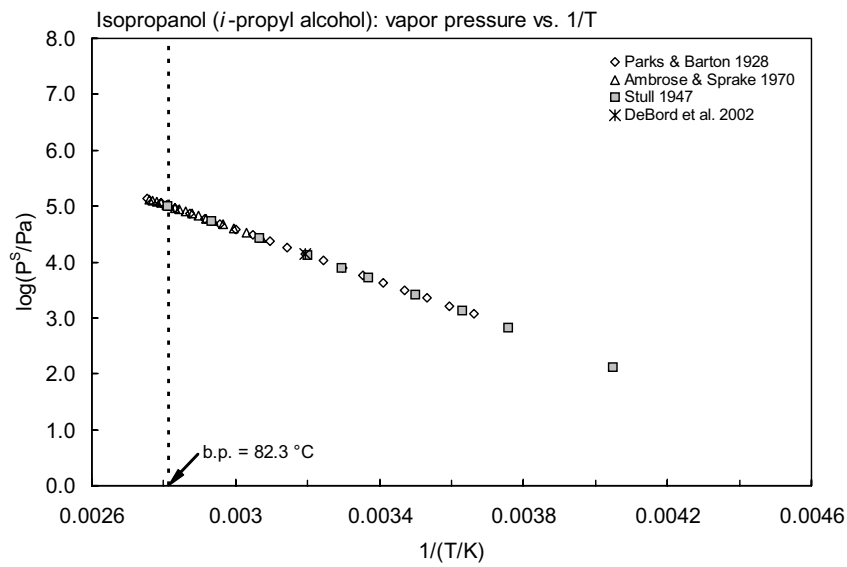✳ DeBord et al. 2002

b.p. = 82.3 °C

FIGURE 11.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for isopropanol.

TABLE 11.1.1.4.2
Reported Henry's law constants and octanol-air partition coefficients of isopropanol at various temperatures

Henry's law constant				log K_{OA}			
Snider & Dawson 1985		Kolb et al. 1992		Cheng et al. 2003		Gruber et al. 1997	
gas stripping-GC		equilibrium headspace-GC		equilibrium headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
0	0.0811	40	3.16	27	2.186	20.29	3.54
25	0.800	60	9.68	32	2.51	30.3	3.27
		70	15.94	37	3.35	40.4	3.04
enthalpy of transfer:		80	25.09	42	4.24	50.28	2.85
$\Delta H/(kJ\ mol^{-1}) = 58.576$							
		ln $(1/K_{AW}) = A - B/(T/K)$					
			$1/K_{AW}$				
		A	−10.6				
		B	−5413				

Isopropanol (*i*-propyl alcohol): Henry's law constant vs. 1/T

FIGURE 11.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for isopropanol.

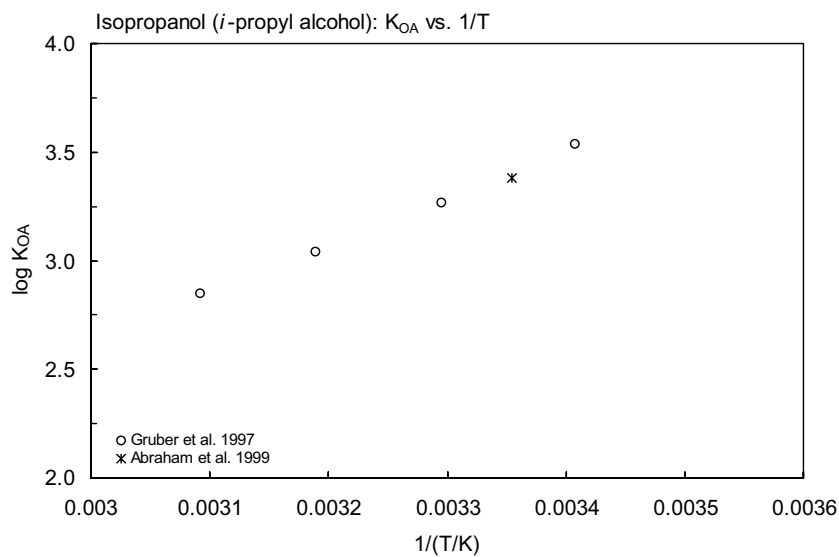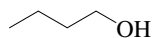Isopropanol (*i*-propyl alcohol): K$_{OA}$ vs. 1/T

FIGURE 11.1.1.4.3 Logarithm of K$_{OA}$ versus reciprocal temperature for isopropanol.

11.1.1.5 *n*-Butanol (*n*-Butyl alcohol)

Common Name: *n*-Butanol
Synonym: 1-butanol, *n*-butyl alcohol, *n*-propylcarbinol
Chemical Name: *n*-butyl alcohol, 1-butanol
CAS Registry No: 71-36-3
Molecular Formula: $C_4H_{10}O$, $CH_3CH_2CH_2CH_2OH$
Molecular Weight: 74.121
Melting Point (°C):
    –88.6   (Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
    117.73   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.80593   (25°C, Butler et al. 1935)
    0.80980   (Weast 1982–83)
    0.80956, 0.80575   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
    91.7   (calculated-density, Rohrschneider 1973)
    103.6   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
    20.89   (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.37   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/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):
    68120, 79000*   (18, 20°C, shake flask-turbidity, Fühner 1924)
    73500*   (volumetric method, Hill & Malisoff 1926)
    64000*   (20°C, synthetic method, Jones 1929)
    70800*   (30°C, vapor liquid equilibrium, measured range 0–105°C, Mueller et al. 1931)
    74500   (gravimetric method, Stockhart & Hull 1931)
    73180   (24.85°C, shake flask-interferometer, Butler et al. 1933)
    73100   (shake flask-cloud point, Butler et al. 1933)
    70000   (26°C, synthetic method, Othmer et al. 1945)
    73320   (shake flask-residue volume, Booth & Everson 1948)
    74100   (shake flask-interferometry, Hansen et al. 1949)
    73000   (shake flask-interferometry, quoted from Butler et al. 1933, Donahue & Bartell 1952)
    75850   (estimated, McGowan 1954)
    78700   (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
    74000   (surface tension, Kinoshita et al. 1958)
    70000   (titration, Petriris & Geankopolis 1959)
    75600*   (20°C, synthetic method, measured range 0–125°C, von Erichsen 1962)
    77800   (shake flask-GC, Korenman et al. 1974, 1975)
    74000*   (shake flask-colorimetric analysis, De Santis et al. 1976)
    70000*   (29.8°C, shake flask-refractometry, measured range 29.8–124.6°C,
      Aoki & Moriyoshi 1978)
    63300   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
    77000   (Verschueren 1983; Howard 1990)
    74000*   (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)
    74500   (selected, Riddick et al. 1986)

80300*　　　(20°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson & Stuart 1986)
74600　　　(selected, Yaws et al. 1990)
65720　　　(shake flask-GC, Li et al. 1992)
71230　　　(shake flask-GC, Li & Andren 1994)

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

800*　　　　(24.0°C, static method, measured range 15.1–117.6°C, Kahlbaum 1898)
904*　　　　(24.98°C, modified isoteniscope method, measured range 24.98–101.16°C, Butler et al. 1935)
$\log (P/\text{mmHg}) = 40.2105 – 4100/(T/K) – 10.35 \cdot \log (T/K)$; temp range 25–110°C (isoteniscope measurements, Butler et al. 1935)
819　　　　　(saturated vapor density-gas saturation, Puck & Wise 1946)
667*　　　　(20°C, summary of literature data, temp range –1.20 to 117°C, Stull 1947)
$\log (P/\text{mmHg}) = 8.27488 – 1873.9/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
10274*　　　(64.56°C, measured range 64.56–117.56°C, Brown & Smith 1959)
820　　　　　(calculated-Antoine eq., Reid & Sherwood 1966)
733*　　　　(22.6°C, ebulliometry-differential thermal analysis, measured range 22.6–117.8°C, Kemme & Kreps 1969)
$\log (P/\text{mmHg}) = 7.42117 – 1351.555/(179.810 + t/°C)$; temp range 22.6–117.8°C, or pressure range 5.5–766 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
910*　　　　(comparative ebulliometry, measured range 78.558–125.686°C, Ambrose & Sprake 1970)
$\log (P/\text{Pa}) = 6.41435 – 1262.767/(T/K – 104.445)$; restricted temp range 78.558–100.74°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
$\log (P/\text{Pa}) = 6.54743 – 1338.769/(T/K – 96.108)$; temp range 78.558–125.686°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
864　　　　　(Hoy 1970)
948*　　　　(298.11 K, measured range 283.10–323.12 K, Geiseler et al. 1973)
$\log (P/\text{mmHg}) = [–0.2185 \times 10970.5/(T/K)] + 8.929597$; temp range –1.2 to 277°C (Antoine eq., Weast 1972–73)
868*　　　　(24.96°C, vapor-liquid equilibrium data, temp range 281.1–323.12 K, Gmehling et al. 1982)
586, 1333　(20°C, 30°C, quoted, Verschueren 1983)
890　　　　　(interpolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.54068 – 1335.018/(176.654 + t/°C)$; temp range 78.56–125.7°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.71950 – 1428.939/(185.552 + t/°C)$; temp range 41.5–108.8°C (Antoine eq. from reported exptl. data Kahlbaum 1898, Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.66896 – 1405.473/(183.866 + t/°C)$; temp range 64.5–117.56°C (Antoine eq. from reported exptl. data of Brown & Smith 1959, Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.7666 – 1460.309/(189.211 + t/°C)$; temp range 22.6–117.8°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
936　　　　　(Daubert & Danner 1985)
824　　　　　(interpolated-Antoine eq., Dean 1985)
$\log (P/\text{mmHg}) = 7.47680 – 1362.39/(178.77 + t/°C)$; temp range 15–131°C (Antoine eq., Dean 1985, 1992)
910　　　　　(selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.54743 – 1338.769/(177.042 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/\text{kPa}) = 6.41661 – 1264.515/(–104.202 + T/K)$; temp range 376–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.54172 – 1336.026/(–96.348 + T/K)$; temp range 323–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.05559 – 1738.4/(–46.544 + T/K)$, temp range: 413–550 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 8.9241 – 2697/(T/K)$; temp range 209–251 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.41594 – 1264.106/(–104.251 + T/K)$; temp range 376–397 K (Antoine eq.-V, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.54723 – 1339.093/(–96.03 + T/K)$; temp range 351–397 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

905* (298.11 K, static method-Hg manometer, measured range 283.10–323.12 K, Gracia et al. 1992)

998 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 39.6673 - 4.0017 \times 10^3/(T/\text{K}) - 10.295 \cdot \log (T/\text{K}) - 3.2572 \times 10^{-10} \cdot (T/\text{K}) + 8.6672 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 184–563 K (vapor pressure eq., Yaws 1994)

933* (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

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

0.866 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

0.731 (entrainment method-GC, Burnett 1963)

0.892 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

0.860; 0.964; 1.057 (exptl.; calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

0.860 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)

4.024* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

$\ln (1/K_{AW}) = -10.2 + 5234/(T/\text{K})$; temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

0.880 (limiting activity coefficient by headspace-GC., Li & Carr 1993)

0.868 (wetted-wall column-GC, Altschuh et al. 1999)

1.214 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

$\ln K_{AW} = 12.141 - 5982.0/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 6.600 - 3009/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.83 (shake flask-CR, Collander 1951)

0.84 (calculated-π constant, Hansch et al. 1968)

0.88 (Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)

0.84, 0.86; 0.84 (calculated-fragment const.; calculated-π constant, Rekker 1977)

0.89 (Hansch & Leo 1979)

0.955 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)

1.02 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)

0.80 (calculated by Rekker's method, Hanai et al. 1981)

0.79 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

0.76 (calculated from measured activity coeff. γ, Wasik et al. 1981)

0.93 (shake flask-RC, Cornford 1982)

0.80 (RP-HPLC-k' correlation, D'Amboise & Hanai 1982)

0.87 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)

0.79 (generator column-GC, Schantz & Martire 1987)

0.80 (calculated from measured activity coeff., γ, Schantz & Martire 1987)

0.87 (calculated-γ from UNIFAC, Banerjee & Howard 1988)

0.823, 0.84 (calculated-CLOGP, calculated-M.O. indices, Bodor et al. 1989)

0.84 (recommended, Sangster 1989, 1993)

0.87 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)

0.89 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

0.88 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log$ BCF:

–0.439 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

    1.85   (calculated-K_{OW}, Lyman et al. 1982)

    0.64   (calculated-MCI χ, Gerstl & Helling 1987)

    0.50   (soil, quoted exptl., Meylan et al. 1992)

    0.39   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

    0.50   (calculated-K_{OW}, Kollig 1993)

    0.50   (soil, calculated-MCI $^1χ$, Sabljic et al. 1995)

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

    Volatilization: evaporation rate k = 2.538×10^{-4} mol m^{-2} h^{-1} was determined by gravimetric method with an air flow rate k = (50 ± 1) L h^{-1} at 20 ± 0.1°C (Gückel et al. 1973);

        estimated half-lives, $t_{1/2}$ ~2.4 h in streams, $t_{1/2}$ ~3.9 h in rivers and $t_{1/2}$ ~125.9 h in lakes (Lyman et al. 1982; quoted, Howard 1990).

    Photolysis:

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

        k = 2.2×10^9 L mol^{-1} s^{-1} for the reaction with 1×10^{-17} M hydroxyl radical in water with $t_{1/2}$ ~1 yr (Anbar & Neta 1967; quoted, Howard 1990)

        photooxidation $t_{1/2}$ = 2602–104000 h in water, based on measured rate constant for reaction with OH radical in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991)

        k_{OH} = 6.8×10^{-10} cm^3 molecule^{-1} s^{-1} at 292 K (relative rate method, Campbell et al. 1976)

        photooxidation $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

        $t_{1/2}$ = 6.5 h for the vapor phase reaction with photochemically produced NO radical in the atmosphere (Dilling et al. 1976; quoted, Howard 1990)

        k_{OH} = 4.1×10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (Lyman et al. 1982)

        k = 0.58 ± 0.06) M^{-1} s^{-1} for the reaction with ozone in water at pH 2.0-6.0 and 20–23°C (Hoigné & Bader 1983)

        k_{OH}(calc) = 6.7×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 7.3×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

        photooxidation $t_{1/2}$ = 8.8–87.7 h in air, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

        estimated half-life of 2.3 d for the vapor phase reaction with photochemically produced OH radical in the atmosphere (GEMS 1986; quoted, Howard 1990)

        k_{OH}(exptl) = 7.3×10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{OH}(calc) = 6.4×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

        k_{OH} = (8.31 ± 0.63) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

        k_{OH}(exptl) = 8.31×10^{-12} cm^3 molecule^{-1} s^{-1} and k(soln) = 7.0×10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with OH radical in aqueous solution (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987b)

        k_{OH} = 8.31×10^{-12} cm^3 molecule^{-1} s^{-1}; k(soln) = 7.0×10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

        k_{OH} = (7.2 - 8.31) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 292–296 K (review, Atkinson 1989)

        k_{OH} = 8.3×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1990)

        k_{OH} = (7.80 ± 0.2) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = (8.56 ± 0.70) $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

        k_{OH}(calc) = 8.9×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

    Hydrolysis:

    Biodegradation:

        $t_{1/2}$(aq. aerobic) = 24–168 h, based on unacclimated freshwater grab sample data (Hammerton 1955) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

        k = 84.0 mg COD g^{-1} h^{-1}, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$(aq. anaerobic) = 96–1296 h, based on acclimated screening test data (Chou et al. 1979; selected, Howard et al. 1991) and aqueous aerobic biodegradation half-life (Howard et al. 1991);

k(calc) = $(0.959 \pm 0.063) \times 10^2$ h^{-1} by activated sludge (Yonezawa & Urushigawa 1979)

k = 0.035–0.046 h^{-1} in 30 mg/L activated sludge after a time lag of 5-10 h (Urano & Kato 1986).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.24-2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2}$ = 6.5 h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

$t_{1/2}$(calc) = 1.2 d for the atmospheric reaction with 1×10^{-6} molecules/cm^3 of OH radical (Howard 1990);

photooxidation $t_{1/2}$ = 8.8-87.7 h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected Howard et al. 1991).

Surface water: $t_{1/2}$ = 24-168 h, based on unacclimated freshwater grab sample data (Hammerton 1955; selected, Howard et al. 1991) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

photooxidation $t_{1/2}$ = 2602-104000 h, based on measured rate constant for reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

estimated volatilization half-lives, $t_{1/2}$ = 2.4 h in streams, $t_{1/2}$ = 3.9 h in rivers and $t_{1/2}$ = 125.9 h in lakes (Lyman et al. 1982; quoted, Howard 1990).

Groundwater: $t_{1/2}$ = 48-1296 h, based on estimated aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:

TABLE 11.1.1.5.1
Reported aqueous solubilities of 1-butanol at various temperatures

1.

Fühner 1924		Hill & Malisoff 1926		Jones 1929		Mueller et al. 1931	
synthetic method		volumetric method		synthetic method		vapor liquid equilibrium	
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	104500	5	95500	0	91000	0	95500
10	90000	10	89100	20.0	64000	15	83000
20	79000	15	82100	40.0	60300	30	70800
30	71000	20	78100	60.0	60000	45	65000
40	65500	25	73500	65.0	60300	60	65200
50	63500	30	70800	80.0	64000	75	68000
60	63500	35	68300	100.0	82000	90	78000
70	65500	40	66000	107.72	97900	105	98000
80	70000	50	64600	110.0	102000		
90	78000	60	65200	120.0	147000		
100	90500	70	67300				
110	10900	80	68900				
		97.9	87400				
		114.5	127300				
		116.9	134600				
		123.3	197300				
		125.15	304400				

(Continued)

TABLE 11.1.1.5.1 *(Continued)*

2.

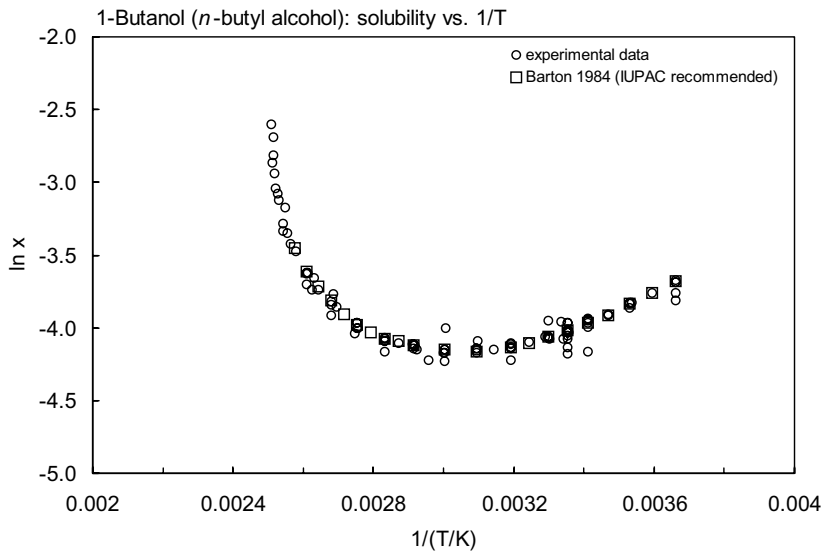| von Erichsen 1952		Aoki & Moriyoshi 1978		Barton 1984		Stephenson & Stuart 1986	
synthetic method		shake flask-refractometry		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
		at 1atm					
0	103200	29.8	70000	0	104000	0	103300
10	86800	49.6	69000	5	96000	9.6	89800
20	75600	59.5	75000	10	89000	20.0	80300
30	70600	69.5	67000	15	82000	30.8	70700
40	67200	89.5	75000	20	78000	40.1	67700
50	65500	99.3	95000	25	74000	50.0	65400
69	65200	106.9	106000	30	71000	60.1	63500
70	66700	109.8	110000	35	68000	70.2	67300
80	69000	118.1	145000	40	66000	80.1	70400
90	75000	119.1	172000	50	64000	90.8	72600
100	88200	122.1	182000	60	65000		
110	110500	122.7	189000	70	67000		
120	154500	123.9	218000	75	69000		
125	235000	124.3	247000	80	70000		
		124.6	279000	85	73000		
				90	77000		
				95	83000		
De Santis et al. 1976				100	91000		
shake flask-colorimetry				105	100000		
				110	111000		
20	80000			115	130000		
30	79400						
40	66000						

FIGURE 11.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.2
Reported vapor pressures of 1-butanol at various temperatures and the coefficients for the vapor pressure equations

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

1.

Kahlbaum 1898		Butler et al. 1935		Stull 1947		Brown & Smith 1959	
static method		isteniscope method		summary of literature data			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
41.5	2866	24.98	904	−1.20	133.3	64.56	10274
44.3	3200	40.0	1276	20.0	666.6	64.74	10371
46.2	3466	45.03	1800	30.2	1333	70.15	13668
48.6	4133	50.08	4593	41.5	2666	75.39	17692
50.1	4400	60.11	8091	53.4	5333	79.00	20982
52.0	5066	70.29	13732	60.3	7999	79.02	21022
55.0	5999	80.58	22465	70.1	13332	89.14	33160
60.2	7999	90.83	35544	84.3	26664	97.33	46859
64.3	9999	101.16	77140	100.8	53329	103.3	59548
69.8	13332			117.5	101325	108.23	72038
78.1	19998	bp/°C	117.71			113.26	86855
84.3	26664	D^{25}	0.8059	mp/°C	−79.9	117.56	131371
89.4	33330						
93.7	39997	eq. 4	P/mmHg				
97.4	46663	A	40.2105				
100.0	53329	B	4100				
103.7	59995	C	10.35				
106.3	66661						
108.8	73327	$\Delta H_V/(kJ\ mol^{-1}) = 52.84$					
		at 25°C					

2.

Kemme & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
22.6	733.3	78.558	20413	283.10	309	283.10	269
30.9	1373	84.243	26518	288.13	457	288.13	405
36.2	1973	89.212	33045	293.12	663	293.12	599
40.7	2613	93.662	39973	298.11	948	298.11	868
48.2	4133	97.357	46601	303.11	1335	303.11	1241
52.4	5280	100.743	53450	308.10	1856	308.10	1744
58.3	7373	103.636	59932	313.08	2545	313.08	2416
65.8	10852	106.367	66630	318.11	3457	318.11	3309
73.5	16185	108.884	73332	323.12	4640	323.12	4473
85.1	27731	111.162	79856				
93.8	40463	113.429	86807	ref. from	Gracia 1989		
196.5	67594	115.324	92996				

(Continued)

TABLE 11.1.1.5.2 (*Continued*)

Kemme & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
117.8	102125	117.413	100142				
		119.193	106702				
Antoine eq.		120.939	113410				
eq. 2	P/mmHg	122.564	119943				
A	7.42117	124.115	126625				
B	1351.864	125.686	133323				
C	179.810						

3.

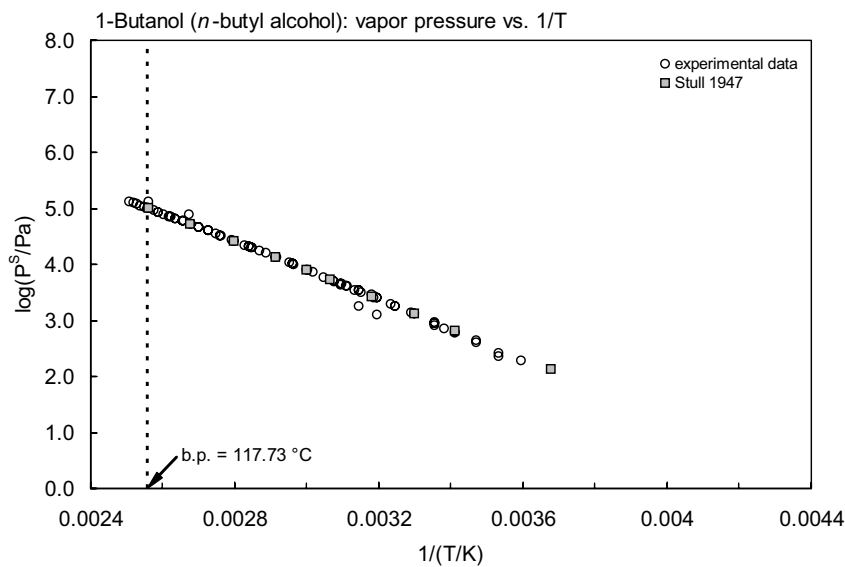| Gracia et al. 1992		Garriga et al. 2002	
static method-Hg manometer		static method-manometer	
T/K	P/Pa	T/K	P/Pa
283.10	265	278.15	192
288.13	411	283.15	230
293.12	613	288.15	453
298.11	905	293.15	635
303.11	1315	298.15	933
308.10	1831	303.15	1315
313.08	2522	308.15	1827
318.11	3420	313.15	2518
323.12	4600	318.15	3429
		323.15	4586
Antoine eq.			
eq. 3a	P/kPa		
A	12.12863		
B	2039.057		
C	132.925		

FIGURE 11.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.3
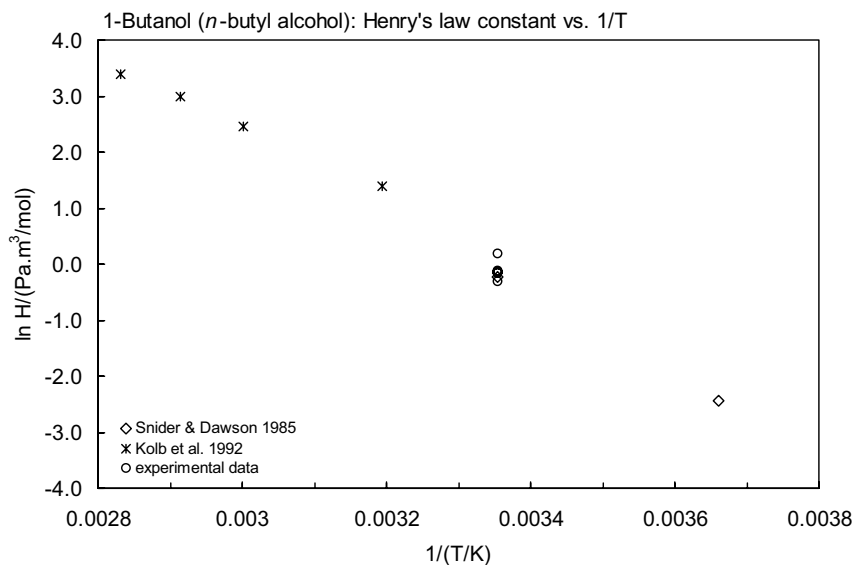**Reported Henry's law constants of 1-butanol at various temperatures and temperature dependence equations**

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

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

$$\ln [H/(atm \cdot m^3/mol)] = A - B/(T/K) \qquad (4a)$$

Snider & Dawson 1985		Kolb et al. 1992	
gas stripping-GC		equilibrium headspace-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
0	0.0873	40	4.024
25	0.800	60	11.64
		70	19.81
enthalpy of transfer:		80	29.69
$\Delta H/(kJ\ mol^{-1}) = 58.576$			
		eq. 2a	$1/K_{AW}$
		A	−10.2
		B	5234

FIGURE 11.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-butanol.

11.1.1.6 Isobutanol (*i*-Butyl alcohol)
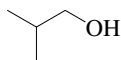
Common Name: Isobutanol
Synonym: isobutyl alcohol, 2-methyl-1-propanol, *i*-butyl alcohol
Chemical Name: isobutanol, isobutyl alcohol, 2-methyl-1-propanol
CAS Registry No: 78-83-1
Molecular Formula: $C_4H_{10}O$, $(CH_3)_2CHCH_2OH$
Molecular Weight: 74.121
Melting Point (°C):
   –101.9   (Lide 2003)
Boiling Point (°C):
   1087.89   (Lide 2003)
Density (g/cm³ at 20°C):
   0.8018   (Weast 1982–83)
   0.8016, 0.7978   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
   92.5   (20°C, calculated-density)
   103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   6.32   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   100140   (18°C, shake flask-turbidity, Fühner 1924)
   85000   (20°C, Seidell 1941)
   75600   (shake flask-interferometry, Donahue & Bartell 1952)
   94000   (shake flask-colorimetric, De Santis et al. 1976)
   95000   (18°C, Verschueren 1983)
   76270   (IUPAC recommended, Barton 1984)
   100000   (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   1541*   (24.98°C, modified isteniscope method, measured range 25–90°C, Butler et al. 1935)
   log (P/mmHg) = 43.5513 – 4185/(T/K) – 11.50·log (T/K); temp range 25–100°C (isteniscope measurements, Butler et al. 1935)
   1648   (interpolated-regression of tabulated data, Stull 1947)
   1333*   (21.7°C, summary of literature data, temp range –9.0 to 108°C, Stull 1947)
   1527*   (comparative ebulliometry, measured range 343.044–388.733 K, Ambrose & Sprake 1970)
   log (P/Pa) = 6.35383 – 1194.628/(T/K – 106.291); restricted temp range 343–367.4 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
   log (P/Pa) = 6.50091 – 1275.197/(T/K – 97.363); temp range 343–388.8 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
   log (P/mmHg) = [–0.2185 × 10936.0/(T/K)] + 9.1138032; temp range –9.0 to 241°C (Antoine eq., Weast 1972–73)
   1527   (selected, Riddick et al. 1986)
   log (P/kPa) = 6.50091 – 1295.197/(t/°C + 175.787), temp range not specified (Riddick et al. 1986)
   log (P_L/kPa) = 6.34528 – 1190.463/(–106.712 + T/K); temp range 369–389 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.49241 – 1271.027/(–97.758 + T/K)$; temp range 313–411 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 7.05055 – 1511.48/(–81.634 + T/K)$; temp range 381–524 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 9.8507 – 2875/(T/K)$; temp range 202–243 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.34606 – 1190.8481/(–106.673 + T/K)$; temp range 369–389 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.50104 – 1275.669/(–97.269 + T/K)$; temp range 342–389 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.27047 – 1147.676/(–111.933 + T/K)$; temp range 383–416 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

log $(P/mmHg) = 109.2803 – 6.306 \times 10^3/(T/K) – 36.947 \cdot log(T/K) + 1.4462 \times 10^{-2} \cdot (T/K) – 3.948 \times 10^{-13} \cdot (T/K)^2$; temp range 165–548 K (vapor pressure eq., Yaws 1994)

1500   (selected, Mackay et al. 1992, 1995)

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

1.20	(measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
1.214	(exptl.-C_W/C_A, Hine & Mookerjee 1975)
1.159. 1.057	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.992	(headspace-GC, Snider & Dawson 1985)
1.186	(calculated-MCI χ, Nirmalakhandan & Speece 1988b)
1.84	(solid-phase microextraction SPME-GC, Bartelt 1997)
2.73	(gas stripping-GC, Shiu & Mackay 1997)
0.892	(wetted-wall column-GC, Altschuh et al. 1999)

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

0.83	(shake flask-CR, Collander 1951)
0.61	(calculated-π constant, Hansch et al. 1968)
0.64	(Leo et al. 1969)
0.65	(from Hansch & Dunn III unpublished result, Leo et al. 1971)
0.76	(shake flask-GC, Dillingham et al. 1973)
0.76	(shake flask, Hansch & Leo 1985; 1987)
0.76	(recommended, Sangster 1989, 1993)
0.76	(recommended, Hansch et al. 1995)

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

3.80   (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization: using Henry's law constant, $t_{1/2}$(calc) = 79.7 h for evaporation from a model river of 1-m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

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

photooxidation $t_{1/2}$ = 201 d to 22 yr in water, based on measured rate for the reaction with OH radical in water (Anbar & Neta 1967; selected, Howard et al. 1991)

photooxidation $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

photooxidation $t_{1/2}$ = 9.96–99.6 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: biodegradation rate constant k = 0.015–0.020 h^{-1} in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986)

$t_{1/2}$(aq. aerobic) = 43–173 h, based on river die-away data for one sample of water from one river (Hammerton 1955; selected, Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 172–692 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition $t_{1/2}$ = 3.5 h under simulated atmospheric conditions, with NO (Dilling et al. 1976); photooxidation $t_{1/2}$ = 9.96–99.6 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation $t_{1/2}$ = 201 d to 22 yr, based on measured rate for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2}$ = 43–173 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 86–346 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 43–173 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

biota:

TABLE 11.1.1.6.1

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

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

Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
24.98	1541	–9.0	133.3	343.044	20457
40.0	2196	11.0	666.6	348.552	26554
45.03	2985	21.7	1333	353.357	33057
50.08	7415	32.4	2666	357.674	39994
60.11	12778	44.1	5333	361.213	46532
70.29	21292	51.7	7999	364.531	53442
80.58	34184	61.5	13332	367.356	59959
90.83	53036	75.9	26664	369.965	66546
		91.4	53329	372.439	73326
bp/°C	82.39	108.0	101325	374.696	79983
D^{25}	0.7812			376.846	86765

(Continued)

TABLE 11.1.1.6.1 (*Continued*)

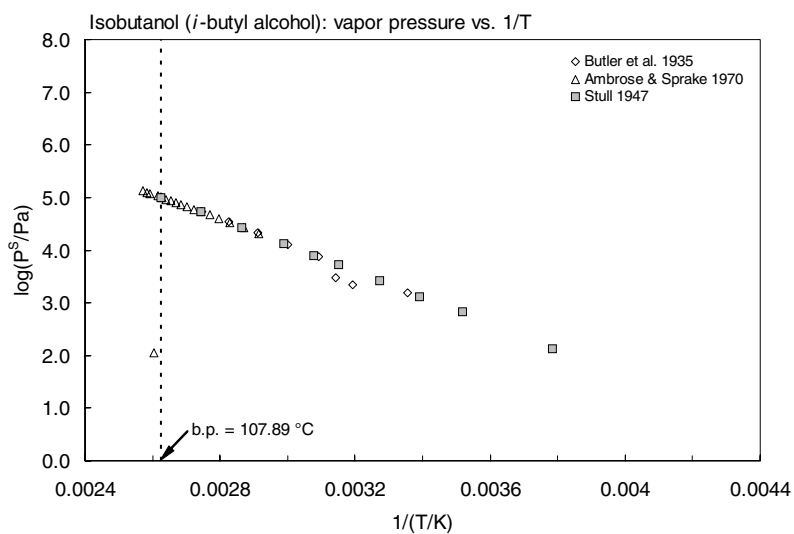| Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
		mp/°C	−108	378.739	93121
eq. 4	P/mmHg			380.718	100153
A	43.5513			382.476	106746
B	4185			384.166	113.417
C	11.50			385.775	120072
$\Delta H_V/(kJ\ mol^{-1}) = 51.63$				387.252	126441
at 25°C				388.773	133283

FIGURE 11.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for isobutanol.

11.1.1.7 *sec*-Butyl alcohol
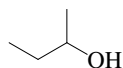
Common Name: *sec*-Butyl alcohol
Synonym: 2-butyl alcohol, 2-butanol, methylethylcarbinol
Chemical Name: 2-butanol, *sec*-butyl alcohol
CAS Registry No: 78-92-2
Molecular Formula: $C_4H_{10}O$, $CH_3CH_2CHOHCH_3$
Molecular Weight: 74.121
Melting Point (°C):
    –88.5   (Lide 2003)
Boiling Point (°C):
    99.51   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8063   (Weast 1982–83)
    0.8065, 0.8024   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    91.9   (20°C, calculated-density)
    103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    200000   (20°C, synthetic method, Jones 1929)
    185000   (20°C, shake flask, Evans 1936)
    198000*   (20°C, shake flask-refractometer, measured range 20–85°C, Morachevskii & Popovich 1965)
    177000, 165000   (25, 35°C, shake flask-titration, Ratouis & Dodé 1965)
    202000*   (20°C, equilibrium pressure cell/shake flask-refractometric method, measured range 10–110°C,
        pressure range 1–800 atm, Moriyoshi et al. 1975)
    225000   (shake flask-colorimetric analysis, De Santis et al. 1976)
    130000   (shake flask-refractometric method, Becke & Quitzch 1977)
    187000*   (equilibrium pressure vessel/shake flask-GC, measured range 265–372 K, pressure range 0.1–75
        MPa, Bozdag & Lamb 1983)
    181000*   (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)
    196000*   (20°C, shake flask-GC/TC, measured range 0–90.2°C, Stephenson & Stuart 1986)
    175340*   (25.28°C, shake flask-laser scattering technique, measured range 276.94–386.6 K, Ochi et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    2286*   (modified isteniscope method, measured range 25–91°C. Butler et al. 1935)
    log (P/mmHg) = 43.4800– 4110/(T/K) – 11.50·log (T/K); temp range 25–90°C (isteniscope measurements,
        Butler et al. 1935)
    2266*   (interpolated-regression of tabulated data, temp range –12.2 to 99.5°C, Stull 1947)
    33031*   (73.392°C, ebulliometry, measured range 73.392–107.146°C, Biddiscombe et al. 1954)
    10610*   (49.730°C, measured range 49.730–99.410°C, Brown et al. 1969)
    2317*   (comparative ebulliometry, measured range 67.723–107.743°C, Ambrose & Sprake 1970)
    log (P/Pa) = 6.26852 – 1126.667/(T/K – 108.361); restricted temp range 67.7–83.34°C (Antoine eq., comparative
        ebulliometry, Ambrose & Sprake 1970)
    log (P/Pa) = 6.86618 – 1360.131/(T/K – 75.558); temp range 67.723–107.743°C (Antoine eq., comparative
        ebulliometry, Ambrose & Sprake 1970)

2357   (Hoy 1970)

log (P/mmHg) = [–0.2185 × 10712.3/(T/K)] + 9.096778; temp range –12.2–251°C (Antoine eq., Weast 1972–73)

1600, 3200   (20°C, 30°C, Verschueren 1983)

2200, 2190, 2275   (extrapolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.35079 – 1169.924/(169.731 + t/°C); temp range 67.7–107.14°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 6.32690 – 1157.363/(168.32 + t/°C); temp range 72.39–107.15°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1954, Boublik et al. 1984)

log (P/kPa) = 6.47826 – 1235.4/(176.82 + t/°C); temp range 49.73–99.41°C (Antoine eq. from reported exptl. data of Brown et al. 1969, Boublik et al. 1984)

2438   (calculated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.47431 – 1314.31/(186.55 + t/°C); temp range 25 to 120°C (Antoine eq., Dean 1985, 1992)

2317   (selected, Riddick et al. 1986)

log (P/kPa) = 6.35457 – 1171.893/(t/°C + 169.955), temp range not specified (Riddick et al. 1986)

log (P_L/kPa) = 6.26823 – 1126.887/(–108.291 + T/K); temp range 359–381 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.34976 – 1169.754/(–103.388 + T/K); temp range 3039–403 K (Antoine eq-II., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.74369 – 735.87/(–176.795 + T/K); temp range 372–5241 K (Antoine eq-III., Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.50959 – 1751.931/(–52.906 + T/K); temp range 210–303 K (Antoine eq-IV., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.2663 – 1125.853/(–108.414 + T/K); temp range 359–380 K (Antoine eq-V., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.35314 – 1171.484/(–103.199 + T/K); temp range 340–379 K (Antoine eq-VI., Stephenson & Malanowski 1987)

2440, 997 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = 49.4476 – 4.2487 × 10³/(T/K) –13.793·log(T/K) + 6.2736 × 10⁻¹¹·(T/K) + 2.1988 × 10⁻⁶·(T/K)²; temp range 158–536 K (vapor pressure eq., Yaws 1994)

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

1.040   (measured partial pressure/mole fraction *x* at dilute concn, Butler 1935)

1.033   (exptl., Hine & Mookerjee 1975)

1.60, 1.057   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.918*   (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

1.107   (calculated-MCI χ, Nirmalakhandan & Speece 1988b)

0.604   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_AW = 6.734 – 3031/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_OW:

0.61   (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)

0.74, 0.64   (calculated-f const., calculated-π const., Rekker 1977)

0.81   (HPLC-RT correlation, Yonezawa & Urushigawa 1979)

0.87   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

0.65   (recommended, Sangster 1989)

0.61   (recommended, Hansch et al. 1995)

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

3.99*   (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

3.80   (calculated from determined γ° in octanol and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

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

        photooxidation $t_{1/2}$ = 129 d to 23 yr, based on measured rate for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

        photooxidation $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

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

        k_{OH} = 4.1×10^9 M^{-1} s^{-1} for at 25°C with $t_{1/2}$ = 1.3 d (Hendry & Kenley 1979; quoted, Mill 1982)

    Hydrolysis:

    Biodegradation: aqueous aerobic $t_{1/2}$ = 24–168 h, based on river die-away studies (Hammerton 1955; selected, Howard et al. 1991) and aqueous anaerobic $t_{1/2}$ = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (selected, Howard et al. 1991);

        average rate of biodegradation k_B = 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)

    Biotransformation:

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

Half-Lives in the Environment:

    Air: photooxidation $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2}$ = 4.0 h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

    photooxidation $t_{1/2}$ = 7.2–72 h, based on measured rate constant for the reaction with OH radical in air (Edney & Corse 1986; selected, Howard et al. 1991);

    calculated lifetimes of 1.3 d and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000)

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

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

    Sediment:

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

    Biota:

TABLE 11.1.1.7.1
Reported aqueous solubilities of *sec*-butyl alcohol at various temperatures

1.

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
			at 1 atm		at 0.1 MPa		
20	198000	10	239000	−8	271000	10	239000
40	146000	20	202000	−6	266000	20	199000
60	140000	27	179000	−4	266000	25	181000
80	140000	40	149000	−3	263000	30	175000

(Continued)

TABLE 11.1.1.7.1 (*Continued*)

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
85	150000	50	132000	0	264000	35	163000
		60	128000	2	256000	40	155000
		70	129000	5	249000	50	140000
		80	138000	10	232000	60	142000
		90	155000	15	228000	70	138000
		100	183000	20	203000	80	143000
		110	239000	25	187000	90	158000
				30	171000	100	186000
		measured range 283–378 K				110	239000
		pressure range 1–800 atm		measured range 265–372 K			
		full list of data see ref.		pressure range 0.1–75 MPa			
				full list of data see ref.			

2.

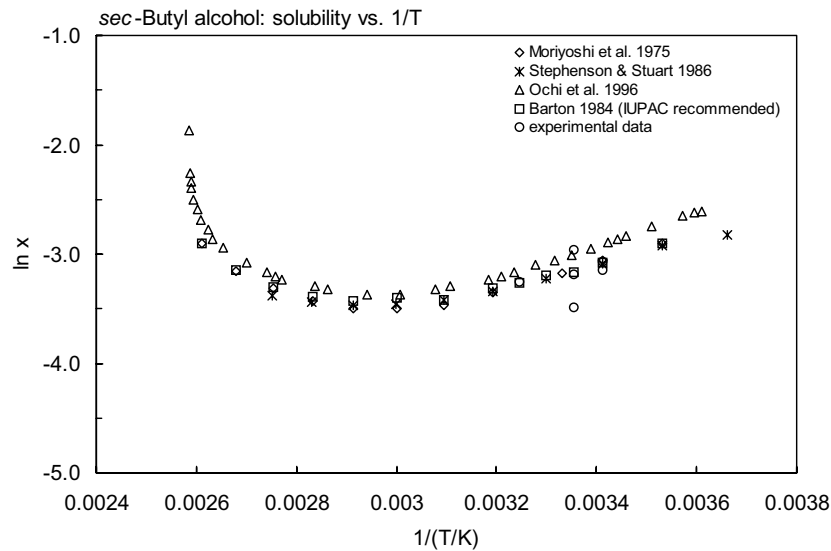| Stephenson & Stuart 1986		Ochi et al. 1996			
shake flask-GC/TC		laser scattering technique			
t/°C	S/g·m⁻³	T/K	mole frac. x	T/K	mole frac. x
0	260000	276.94	0.0738	362.51	0.0406
10	235000	278.13	0.0725	364.96	0.0421
20	196000	279.96	0.0705	370.41	0.0459
29.9	170000	284.94	0.0642	376.89	0.0530
40	151000	289.08	0.0590	379.76	0.0573
50	140000	290.58	0.0571	381.25	0.0621
60.3	134000	292.18	0.0553	383.23	0.0680
70.1	133000	295.15	0.0522	384.39	0.0751
80.1	136000	298.43	0.0491	385.63	0.0820
90.2	145000	301.48	0.0471	386.04	0.0908
		305.14	0.0452	386.23	0.0965
		309.16	0.0421	386.58	0.1050
		311.88	0.0406	386.65*	0.1151
		314.10	0.0393	*the upper critical solution point	
		321.88	0.0371		
		324.99	0.0361		
		332.50	0.0342		
		340.01	0.0342		
		349.30	0.0361		
		352.25	0.0371		
		360.81	0.0393		

FIGURE 11.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *sec*-butyl alcohol.

TABLE 11.1.1.7.2

Reported vapor pressures of *sec*-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(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.

Butler et al. 1935		Stull 1947		Biddiscombe et al. 1954		Brown et al. 1969	
isteniscope method		summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	2286	–12.2	133.3	73.392	33031	49.730	10610
40.0	3272	7.20	666.6	76.600	39942	54.050	13402
45.03	4440	16.9	1333	80.131	46616	57.740	16271
50.08	10764	27.3	2666	83.340	53447	62.020	20198
60.12	18452	38.1	5333	86.112	39983	67.498	16382
70.3	29878	45.2	7999	88.693	66641	72.180	32861
80.59	47356	54.1	13332	91.068	73266	76.970	40792
90.84	72407	67.9	26664	93.303	80010	83.060	53067
		83.9	53329	95.394	86761	88.450	66274
bp/°C	99.95	99.5	101325	97.252	93093	94.160	83033
D²⁵	0.8029			99.201	100155	99.410	101321
		mp/°C	–114.7	100.931	106774		
eq. 4	P/mmHg			120.611	113533		
A	43.4800			104.186	120168		
B	4110			105.647	126596		
C	11.50			107.146	133.471		

$\Delta H_V/(\text{kJ mol}^{-1}) = 50.21$
at 25°C

TABLE 11.1.1.7.2 *(Continued)*

2.

Ambrose & Sprake 1970

comparative ebulliometry

| t/°C	P/Pa
67.723	26556
72.392	33031
76.601	39942
80.131	46616
83.340	53447
86.111	59984
88.693	66641
91.067	73284
93.303	81010
95.394	86759
97.253	93095
99.201	100154
100.931	106775
102.611	113530
104.186	120167
105.647	126593
107.143	133470
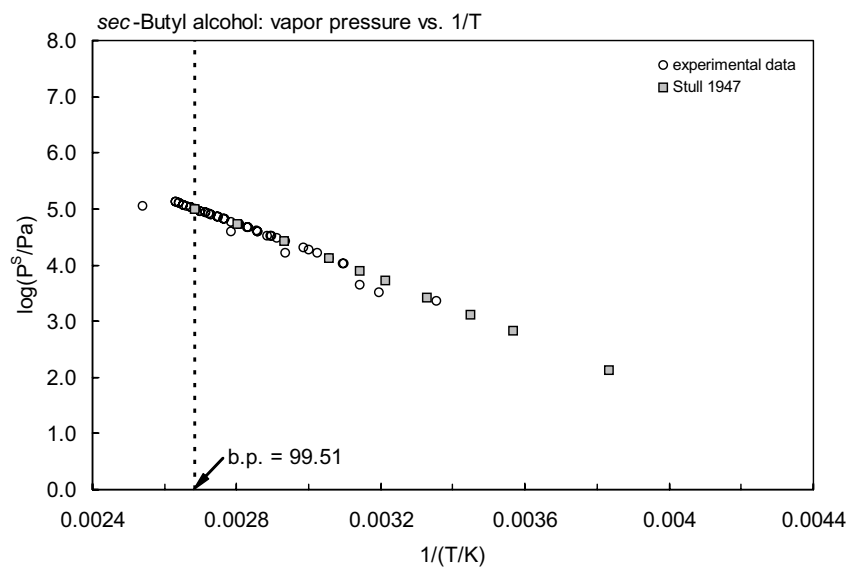
FIGURE 11.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for *sec*-butyl alcohol.

TABLE 11.1.1.7.3

Reported Henry's law constants and octanol-air partition coefficients of *sec*-butyl alcohol at various temperatures

Henry's law constant		log K_{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
0	0.0987	20.29	3.98
25	0.9180	30.3	3.68
		40.4	3.44
enthalpy of transfer:		50.28	3.22
ΔH/(kJ mol⁻¹) = 58.576			
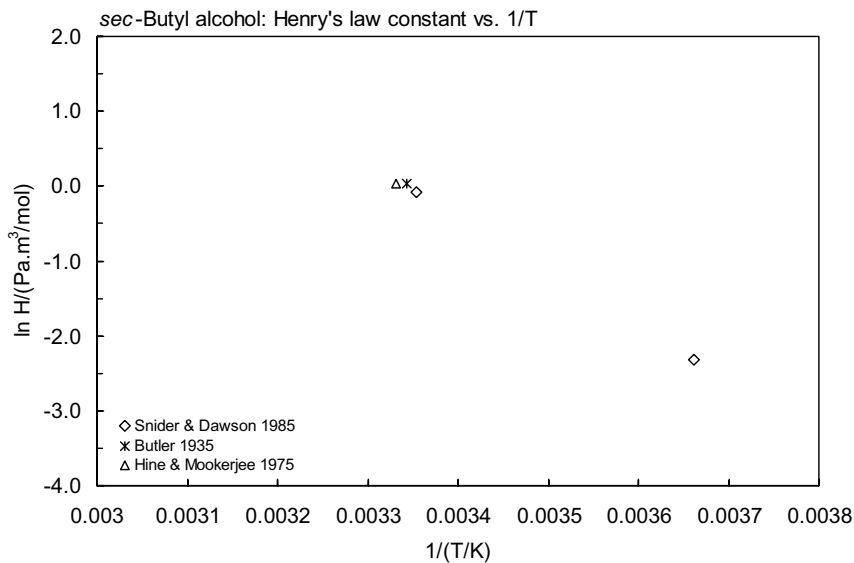
FIGURE 11.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for *sec*-butyl alcohol.
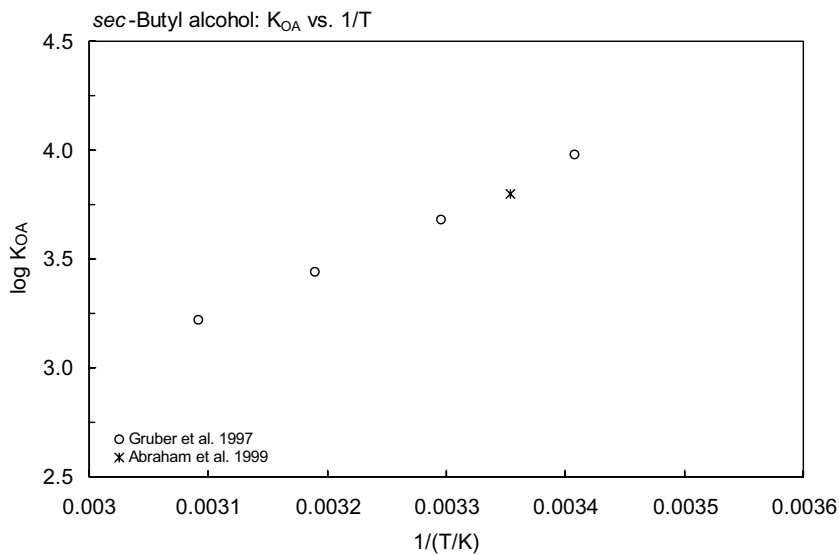
FIGURE 11.1.1.7.4 Logarithm of K_{OA} versus reciprocal temperature for *sec*-butyl alcohol.

11.1.1.8   *tert*-Butyl alcohol

Common Name: *tert*-Butyl alcohol
Synonym: 3-butanol, *t*-butyl alcohol, 2-methyl-2-propanol, trimethylcarbinol,
Chemical Name: *t*-butanol, *t*-butyl alcohol, 2-methyl-2-propanol
CAS Registry No: 75-65-0
Molecular Formula: $C_4H_{10}O$, $(CH_3)_3COH$
Molecular Weight: 74.121
Melting Point (°C):
    25.69   (Lide 2003)
Boiling Point (°C):
    82.4   (Lide 2003)
Density (g/cm³ at 20°C):
    0.78581, 0.78086   (20°C, 25°C, Dreisbach & Martin 1949)
    0.7883   (Weast 1982–83)
    0.7858   (Dean 1985)
    0.7812   (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    94.2   (calculated-density, Rohrschneider 1973)
    103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.64   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    22.76, 56   (observed, estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming $\Delta S = 56$ J/mol K), F: 1.0

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

    miscible (Palit 1947; Riddick et al. 1986)
    miscible (Barton 1984; Dean 1985; Howard 1990; Yaws et al. 1990)
    miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    5600*   (static method/isoteniscope, measured range 20–90°C, Parks & Barton 1928)
    5654*   (24.98°C, modified isoteniscope method, measured range 30–80°C, Butler et al. 1935)
    log (P/mmHg) = 43.2834 – 3935/(T/K) –11.50·log (T/K); temp range 30–80°C (isoteniscope measurements,
        Butler et al. 1935)
    5019*   (interpolated-regression of tabulated data, temp range –20.4 to 82.9°C, Stull 1947)
    log (P/mmHg) = 8.24380 – 1675.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    16500*   (43.34°C, measured range 43.34–82.41°C, Dreisbach & Shrader 1949)
    5637*   (comparative ebulliometry, measured range 329.946–362.710 K, Ambrose & Sprake 1970)
    log (P/Pa) = 6.24072 – 1049.320/(T/K – 107.724); restricted temp range 329.946–345.288 K (Antoine eq.,
        comparative ebulliometry, Ambrose & Sprake 1970)
    log (P/Pa) = 6.35648 – 1107.060/(T/K – 101.048); temp range 329.946–362.71 K (Antoine eq., comparative
        ebulliometry, Ambrose & Sprake 1970)
    log (P/mmHg) = [–0.2185 × 10413.2/(T/K)] + 9.193472; temp range –20.4 to 222.5°C (Antoine eq., Weast
        1972–73)
    5600   (Verschueren 1983; Howard et al. 1986)
    5637   (selected, Riddick et al. 1986)
    log (P/kPa) = 6.35648 – 1107.060/(t/°C + 172.102) temp not specified (Riddick et al. 1986)
    log (P_L/kPa) = 6.22619 – 1042.416/(–108.5 + T/K); temp range 347–363 K (Antoine eq.-I, Stephenson &
        Malanowski 1987)

log $(P_L/kPa) = 6.35045 - 1104.341/(-101.315 + T/K)$; temp range 299–375 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.27388 - 989.74/(-124.966 + T/K)$; temp range 356–480 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.23125 - 1044.891/(-108.211 + T/K)$, temp range: 347–363 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.35498 - 1106.556/(-101.071 + T/K)$; temp range 329–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.09542 - 975.944/(-116.864 + T/K)$; temp range 357–461 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

1008, 5600   (calculated-solvatochromic parameters, quoted lit., Banerjee et al. 1990)

log $(P/mmHg) = 71.8181 - 4.9966 \times 10^3/(T/K) - 21.805 \cdot \log(T/K) + 1.9238 \times 10^{-8} \cdot (T/K) + 5.8247 \times 10^{-6} \cdot (T/K)^2$; temp range 299–506 K (vapor pressure eq., Yaws 1994)

5610*   (static method-manometer, measured range 298.15–323.15 K, Garriga et al. 2002)

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

1.210   (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

1.214   (exptl., Hine & Mookerjee 1975)

1.057, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.460*   (25°C headspace-GC, measured range 0–25°C, Snider & Dawson 1985)

1.426   (calculated-MCI χ, Nirmalakhandan & Speece 1988b)

0.917   (wetted-wall column-GC, Altschuh et al. 1999)

0.907   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log $K_{AW} = 8.467 - 3488/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.37   (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969)

0.59   (HPLC-RT correlation, Yonezawa & Urushigawa 1979)

0.35   (Hansch & Leo 1985)

0.40   (calculated-solvatochromic parameters, Taft et al. 1985)

0.39   (HPLC-k' correlation, Funasaki et al. 1986)

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

0.35   (recommended, Sangster 1989)

0.34   (calculated-UNIFAC activity coefficient, Dallos et al. 1993)

0.35   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

–1.46   (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.57   (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: estimated half-lives, $t_{1/2}$ = 51.6 h in streams, $t_{1/2}$ = 65.37 h in rivers and $t_{1/2}$ = 3104.3 h in lakes were estimated by using Henry's law constant and assuming the wind velocity to be 3 m/s, the current velocities of the streams, rivers, and lakes 2,1, and 0.01 m/s with depths of lakes 50 m and that of the streams and lakes 1 m deep (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

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

photooxidation $t_{1/2}$ = 771 d to 64500 yr, based on measured rate for the reaction with hydroxyl radical in water (Howard et al. 1991)

photooxidation $t_{1/2}$ > 9.9 d(Darnall et al. 1976)

k ~ 0.003 M^{-1} s^{-1} for the reaction with ozone in water at pH 2–6 and 20–23°C (Hoigné & Bader 1983)

k_{OH}(calc) = 6.9 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.09 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2}$ = 59–590 h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

k_{OH}(calc) = 5.9 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1}, and k_{OH}(exptl) = 1.09 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH} = (1.08 ± 0.11) × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

k_{OH} = 1.07 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 1.0 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}* = 1.07 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 243–440 K (flash photolysis-resonance fluorescence, Wallington 1988c)

k_{OH}* = 1.12 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

k(aq.) = 0.01 M^{-1} s^{-1} at pH 2.3, k = 0.45 M^{-1} s^{-1} at pH 2.2, k = 0.46 M^{-1} s^{-1} at pH 5.2 for direct reaction with ozone in water and 20°C, with $t_{1/2}$ = 390 d at pH 7 (Yao & Haag 1991).

k_{OH}(calc) = 0.53 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation 30.0 mg COD g^{-1} h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$(aq. aerobic) = 677–4320 h, based on river die-away studies; $t_{1/2}$(aq. anaerobic) = 2400–12000 h, based on degradation rates in microcosm studies simulating anaerobic aquifers (Howard et al. 1991).

$t_{1/2}$(aerobic) = 28 d, $t_{1/2}$(anaerobic) = 100 d in natural waters (Capel & Larson 1995)

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ > 9.9 d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2}$ = 34.5 h for 10 ppm in the air reacted with 5 ppm NO (Dilling et al. 1976);

photooxidation $t_{1/2}$ = 59-590 h, based on measured rate for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

$t_{1/2}$ ~ 1.09 month for the vapor phase reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2}$ ~ 8.8 yr, based on rate constant k = 2.5 × 10^8 L/mol·s for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard 1990);

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

measured rate constant k = 0.001 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.3 and 20°C, with $t_{1/2}$ = 390 d at pH 7 (Yao & Haag 1991)

$t_{1/2}$(aerobic) = 28 d, $t_{1/2}$(anaerobic) = 100 d in natural waters (Capel & Larson 1995)

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

Sediment:

Soil: $t_{1/2}$ = 360-4800 h, based on soil microcosm studies (Howard et al. 1991).

Biota:

TABLE 11.1.1.8.1

Reported vapor pressures of *tert*-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

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

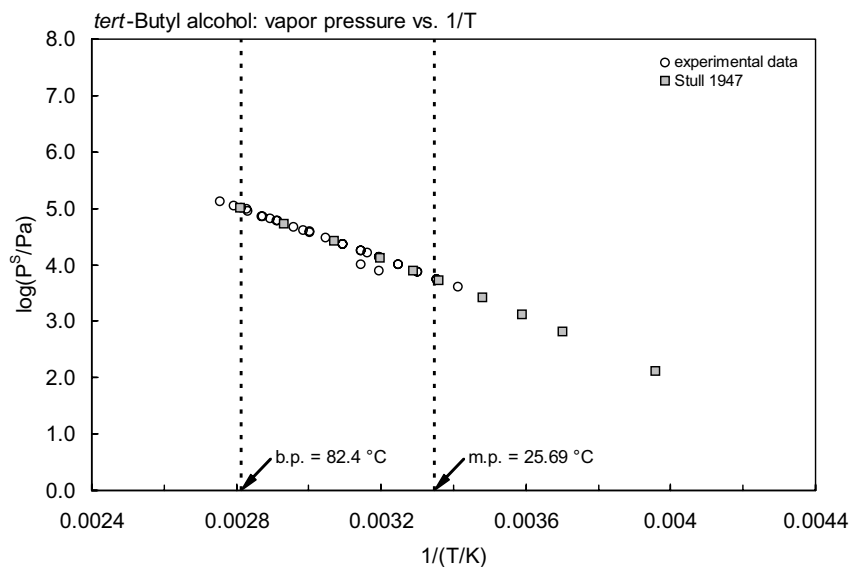| Parks & Barton 1928		Butler et al. 1935		Stull 1947		Garriga et al. 2002	
static method/isoteniscope		isoteniscope method		summary of literature data		static method-manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	4080	24.98	5654*	–20.4	133.3	25	5610
25	5600	40.0	7753	–3.0	666.6	30	7685
30	7586	45.03	10423	5.5	1333	35	10347
35	10172	50.08	23705	14.3	2666	40	13787
40	13639	60.12	38850	24.5	5333	45	18143
45	17839	70.3	61648	31.0	7999	50	23578
50	23238	75.43	72927	39.8	13332		
55	29891	80.59	100112	52.7	26664	**Ambrose & Sprake 1970**	
60	38024		*solid	68.0	53329	comparative ebulliometry	
65	47756	bp/°C	82.75	82.9	101325	T/K	P/Pa
70	59635					329.946	33123
75	73754	eq. 4	P/mmHg	mp/°C	25.3	333.931	40058
80	90579	A	43.2834			337.204	46623
85	110164	B	3935			340.225	53431
90	132816	C	11.59			342.857	60007
						347.448	73160
				Dreisbach & Shrader 1949		351.659	86911
$\Delta H_V/(kJ\ mol^{-1}) =$		$\Delta H_V/(kJ\ mol^{-1}) = 46.86$		ebulliometry		355.146	99932
at 25°C	45.56	at 25°C		t/°C	P/Pa	358.422	113545
at bp	39.66			43.34	16500	362.710	133505
				61.82	42066	full list of data see ref.	
				72.49	67661		
				82.41	101325		

FIGURE 11.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for *tert*-butyl alcohol.

TABLE 11.1.1.8.2
Reported Henry's law constants of *tert*-butyl alcohol at various temperatures

Snider & Dawson 1985	
gas stripping-GC	
t/°C	**H/(Pa m³/mol)**
0	0.1135
25	1.4581

enthalpy of transfer:
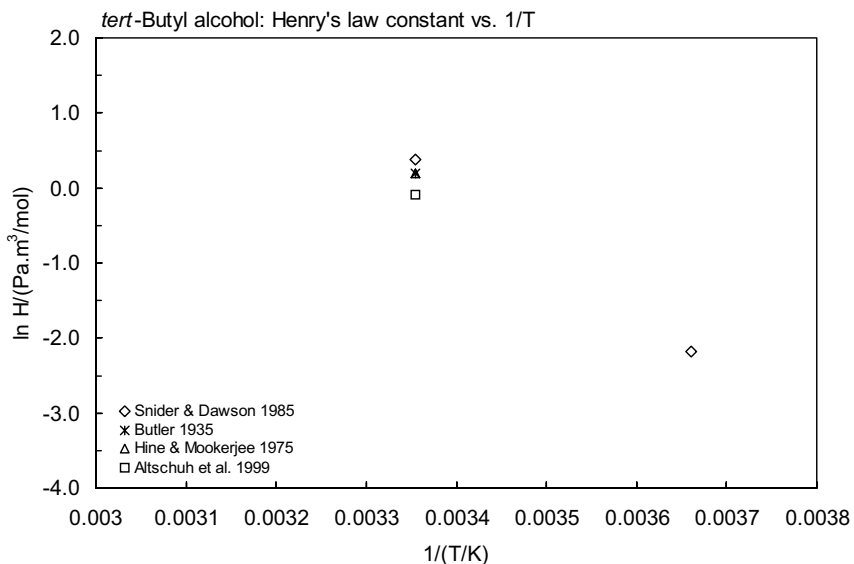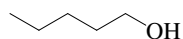 $\Delta H/(\text{kJ mol}^{-1}) = 66.944$

FIGURE 11.1.1.8.2 Logarithm of Henry's law constant versus reciprocal temperature for *tert*-butyl alcohol.

11.1.1.9   1-Pentanol (*n*-Amyl alcohol)

Common Name: 1-Pentanol
Synonym: amyl alcohol, *n*-butylcarbinol, 1-pentanol, *n*-pentyl alcohol, pentyl alcohol
Chemical Name: *n*-amyl alcohol, *n*-pentyl alcohol, 1-pentanol
CAS Registry No: 71-41-0
Molecular Formula: $C_5H_{12}O$, $CH_3CH_2CH_2CH_2CH_2OH$
Molecular Weight: 88.148
Melting Point (°C):
    –77.6   (Lide 2003)
Boiling Point (°C):
    137.98   (Lide 2003)
Density (g/cm³ at 20°C):
    0.81253   (25°C, Butler et al. 1935)
    0.8144   (Weast 1982–83)
    0.81445, 0.81080   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    108.0   (calculated-density, Lande & Banerjee 1981)
    125.8   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
    20.81   (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    10.5   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    22080   (shake flask-interferometer, Butler et al. 1933)
    21900*   (volumetric method, measured range 20–30°C, Ginnings & Baum 1937)
    22100   (20°C, surface tension, Addison 1945)
    23600   (20°C, Seidell 1941)
    27570   (shake flask-residue volume, Booth & Everson 1948)
    15230   (20°C, shake flask-turbidity, Laddha & Smith 1948)
    25400   (shake flask-interferometry, Hansen et al. 1949)
    23500*   (20°C, synthetic method, measured range 0–180°C, von Erichsen 1952)
    22000   (shake flask-titration, Crittenden & Hixon 1954)
    22140   (estimated, McGowan 1954)
    22000   (surface tension, Kinoshita et al. 1958)
    23800   (shake flask-GC, Korenman 1974, 1975)
    21950   (Riddick & Bunger 1955)
    18800   (shake flask-GC, Evans et al. 1978)
    11720   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
    22000*   (recommended best value, IUPAC Solubility Data Series, temp range 0–180°C, Barton 1984)
    22500*   (20.2°C, shake flask-GC/TC, measured range 0–90.7°C, Stephenson et al. 1984)
    20190   (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    333*   (25°C, extrapolated-modified isoteniscope method, measured range 60–131°C, Butler et al. 1935)

log (P/mmHg) = 46.4925 –4580/(T/K) – 12.42·log (T/K); temp range 60–131°C (isoteniscope measurements, Butler et al. 1935)

349*   (interpolated-regression of tabulated data, temp range 13.6–138°C, Stull 1947)

286*   (extrapolated-ebulliometry, measured range 33.9–138°C, Kemme & Kreps 1969)

573.3*   (33.9°C, ebulliometry-differential thermal analysis, measured range 33.9–138°C, Kemme & Kreps 1969)

log (P/mmHg) = 7.55787 – 1492.549/(181.529 + t/°C); temp range 33.9–138°C, or pressure range 4.3–765.4 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

293*   (comparative ebulliometry, measured range 74.763–156°C, Ambrose & Sprake 1970)

log (P/Pa) = 6.13796 – 1190.412/(T/K – 123.055); restricted temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.30306 – 1286.333/(T/K – 111.843); temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

313   (calculated-Antoine eq., Riddick & Bunger 1970)

log (P/mmHg) = [–0.2185 × 12495.5/(T/K)] + 9.574342; temp range 13.6–137.8°C (Antoine eq., Weast 1972–73)

189   (20°C, extrapolated-Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

373   (20°C, Verschueren 1983)

172, 250   (extrapolated-Antoine equations., Boublik et al. 1984)

log (P/kPa) = 6.00024 – 1103.91/(138.221 + t/°C); temp range 165–240.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.31559 – 1292.273/(161.837 + t/°C); temp range 74.5–156°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

313   (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.17758 – 1314.56/(168.11 + t/°C); temp range 37–138°C (Antoine eq., Dean 1985, 1992)

293   (selected, Riddick et al. 1986)

log (P/kPa) = 6.30306 – 1286.333/(t/°C + 161.307), temp range not specified (Riddick et al. 1986)

log (P$_L$/kPa) = 6.14668 – 1195.924/(–122.348 + T/K); temp range 388–420 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.30990 – 1290.23/(–111.419 + T/K); temp range 347–429 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.1490 – 1197.233/(–122.194 + T/K); temp range 388–420 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.3975 – 1337.613/(–106.567 + T/K); temp range 326–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.28069 – 1277.413/(–112.34 + T/K); temp range 408–441 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P/mmHg) = 71.2535 – 5.4977 × 10^3/(T/K) –21.366·log(T/K) + 3.8108 × 10^{-10}·(T/K) + 5.0339 × 10^{-6}·(T/K)^2; temp range 196–586 K (vapor pressure eq., Yaws 1994)

891   (40°C, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)

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

1.324   (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

1.271   (exptl., Hine & Mookerjee 1975)

1.426, 1.60   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.04   (calculated-P/C, Mackay & Yuen 1983)

1.017   (limiting activity coefficient by headspace-GC., Abraham et al. 1987)

1.271   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

1.236   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

1.60   (correlated-molecular structure, Russell et al. 1992)

1.186   (limiting activity coefficient by headspace-GC., Li & Carr 1993)

1.057   (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

ln K$_{AW}$ = 14.233 – 6559.6/(T/K); temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, log K$_{OW}$:

1.40   (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Dunn III 1972)

1.37, 1.38; 1.34   (calculated-fragment const.; calculated-π constant, Rekker 1977)
1.44, 1.48   (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
1.53   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
1.33   (HPLC-RT correlation, D'Amboise & Hanai 1982)
1.56   (shake flask, Log P Database, Hansch & Leo 1987)
1.49   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
1.53   (generator column-GC, Schantz & Martire 1987)
1.55   (calculated from measured γ, Schantz & Martire 1987)
1.51   (recommended value, Sangster 1989, 1993)
1.41   (shake flask-GC, Fujiwara et al. 1991)
1.56   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
    0.241   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:
    0.93   (calculated-MCI χ, Gerstl & Helling 1987)
    0.70   (soil, quoted exptl., Meylan et al. 1992)
    0.65   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
    0.70   (soil, calculated-MCI ^{1}χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
    Volatilization: evaporation rate of 6.92×10^{-5} mol cm^{-2} h^{-1} was determined by gravimetric method with an air flow rate of (50 ± 1) L h^{-1} at $20 \pm 0.1°C$ (Gückel et al. 1973).
    Photolysis:
    Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures see reference:
        photooxidation $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)
        k_{OH}(exptl) = 1.08×10^{-11} cm^3 molecule^{-1} s^{-1}, k = 6.50×10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with hydroxyl radical in aqueous solution at 298 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987)
        k_{OH} = 1.08×10^{-11} cm^3 molecule^{-1} s^{-1}; k(soln) = 6.5×10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
        k_{OH} = 10.8×10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K (review, Atkinson 1989)
        k_{OH} = $(12.0 \pm 1.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; k_{OH} = $(10.5 \pm 1.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)
        k_{OH}(calc) = 9.37×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)
    Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
    Air: $t_{1/2}$ = 0.24–2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).
    Surface water:
    Groundwater:
    Sediment:
    Soil:
    Biota:

TABLE 11.1.1.9.1
Reported aqueous solubilities of 1-pentanol at various temperatures

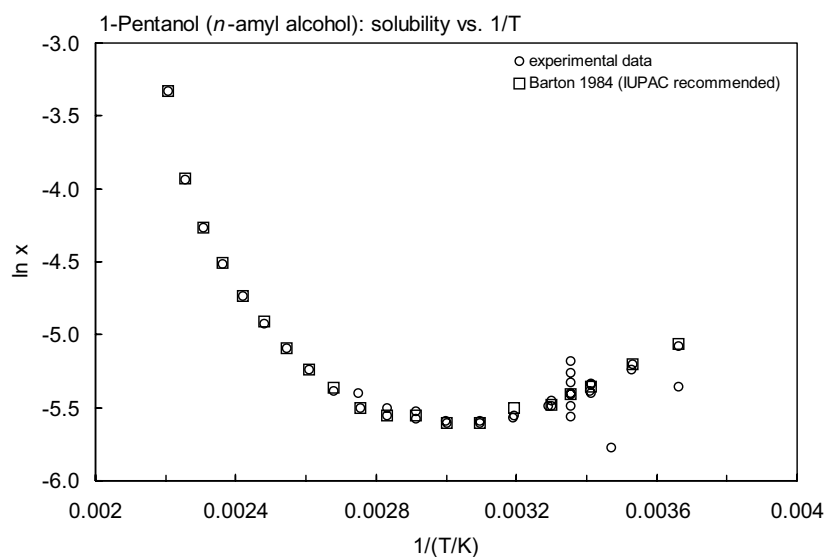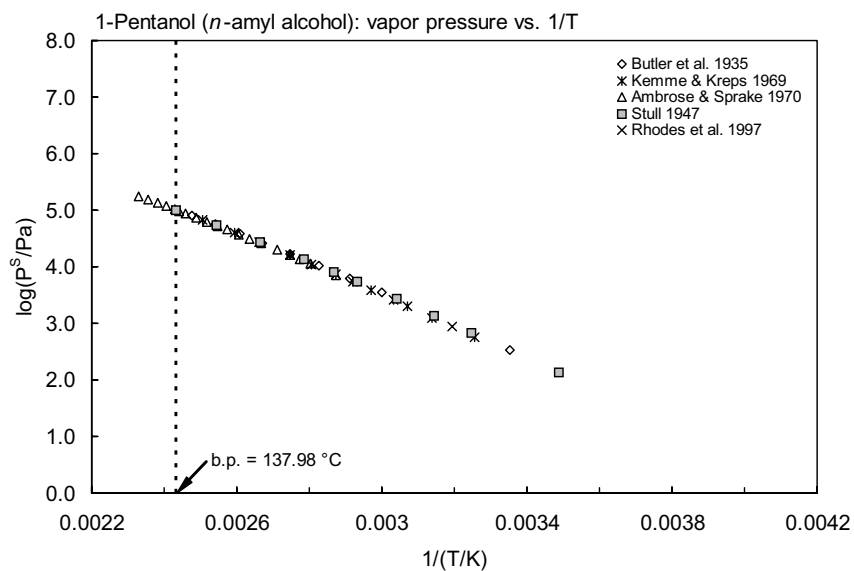| Ginnings & Baum 1937		von Erichsen 1952		Barton 1984		Stephenson et al. 1984	
volumetric method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
20	23600	0	30500	0	31000	0	23100
25	21900	10	27000	10	27000	10.2	25900
30	20300	20	23500	20	23100	20.2	22500
		30	21000	25	22000	30.6	20200
		40	19000	30	20400	40.2	18700
		50	18000	40	20000	50.0	18300
		60	18000	50	18000	60.3	18300
		70	18500	60	18000	70.0	19500
		80	19000	70	19000	80.0	19900
		90	20000	80	19000	90.7	22100
		100	22500	90	20000		
		110	26000	100	23000		
		120	30000	110	26000		
		130	35500	120	30000		
		140	43000	130	36000		
		150	53500	140	43000		
		160	69000	150	54000		
		170	95500	160	69000		
		180	175000	170	96000		
				180	175000		

FIGURE 11.1.1.9.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-pentanol.

TABLE 11.1.1.9.2

**Reported vapor pressures of 1-pentanol at various temperatures and the coefficients for the vapor pressure equations**

$\log P = A - B/(T/K)$	(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)		

Butler et al. 1935		Stull 1947		Kemme & Kreps 1969		Ambrose & Sprake 1970	
isoteniscope method		summary of literature data		differential thermal analysis		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	333.3	13.6	133.3	33.9	573.3	74.763	7175
60.12	3468	34.7	666.6	45.6	1267	83.542	11204
70.3	6153	44.9	1333	52.6	2027	87.571	13615
80.59	10364	55.8	2666	56.7	2640	90.768	15825
90.84	16772	68.0	5333	63.6	3920	95.514	19660
101.17	26398	75.5	7999	69.3	5426	101.629	25714
110.2	38250	85.8	13332	74.9	7306	106.362	31393
120.56	56542	102.0	26664	83.1	11026	110.658	37413
130.89	81580	119.8	53329	90.7	15879	115.564	45399
		137.8	101325	102.4	26664	119.681	53129
bp/°C	137.75			112.3	40263	124.099	62576
D^{25}	0.8125	mp/°C	-	125.8	66941	128.665	73706
				138.0	102045	133.309	86610
eq. 4	P/mmHg					136.688	97054
A	46.4925			Antoine eq.		138.514	103110
B	4580			eq. 2	P/mmHg	142.435	117105
C	11.42			A	7.55787	146.598	133550
				B	1492.549	151.332	154379
$\Delta H_V/(kJ\ mol^{-1}) = 56.90$				C	181.529	155.977	177156
at 25°C							

Antoine eq. for full range

eq. 3	P/mmHg
A	6.30306
B	1286.333
C	111.843

Data also fitted to Cragoe equation, see ref.

FIGURE 11.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1-pentanol.

11.1.1.10   1-Hexanol
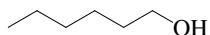
Common Name: 1-Hexanol
Synonym: amylcarbinol, 1-hexanol, *n*-hexyl alcohol
Chemical Name: *n*-hexyl alcohol, 1-hexanol
CAS Registry No: 111-27-3
Molecular Formula: $C_6H_{14}O$, $CH_3CH_2CH_2CH_2CH_2CH_2OH$
Molecular Weight: 102.174
Melting Point (°C):
    –47.4   (Lide 2003)
Boiling Point (°C):
    157.6   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8136   (Weast 1982–83)
    0.81875, 0.81534   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    126.0   (calculated-density, Lande & Banerjee 1981)
    148.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    15.40   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    5000*   (20°C, shake flask-turbidity, measured range 0–110°C, Fühner 1924)
    6240   (shake flask-interferometer, Butler et al. 1933)
    5025   (20°C, shake flask-turbidity, Laddha & Smith 1948)
    6400*   (20°C, synthetic method, measured range 0–220°C, von Erichsen 1952)
    6000   (shake flask-titration, Crittenden & Hixon 1954)
    6300   (estimated, McGowan 1954)
    6000   (surface tension, Kinoshita et al. 1958)
    5838*   (shake flask-refractive index, measured range 5.5–33.6°C, Hill & White 1974)
    3590   (shake flask-GC, Korenman et al. 1974)
    4230   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
    6000*   (recommended best value, IUPAC Solubility Series, temp range 0–220°C, Barton 1984)
    6660*   (20°C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson et al. 1984)
    5354   (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    95.86*   (24.98°C, extrapolated-modified isoteniscope data, measured range 60.11–152.77°C, Butler et al. 1935)
    log (P/mmHg) = 51.0030 – 5068/(T/K) – 13.80·log (T/K), temp range 60–152°C (isoteniscope measurements, Butler et al. 1935)
    151.1*   (interpolated-regression of tabulated data, temp range 24.4–157°C, Stull 1947)
    88.25   (extrapolated, ebulliometry, measured range 52–157°C, Kemme & Kreps 1969)
    760*   (52.2°C, ebulliometry-differential thermal analysis, measured range 52.3–157.3°C, Kemme & Kreps 1969)
    log (P/mmHg) = 7.28781 – 1422.031/(t/°C + 165.444); temp range 52–157°C or pressure range 5.7–757.3 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
    log (P/mmHg) = [–0.2185 × 12708.5/(T/K)] + 9.367617; temp range 24.4–157°C (Antoine eq., Weast 1972–73)

130.6   (20°C, Verschueren 1983)

79.65, 79.7 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.20107 – 1305.63/(153.901 + t/°C)$; temp range 52.2–157.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.26314 – 1334.63/(156.297 + t/°C)$; temp range 60.11–152.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

55.5   (extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

52.9, 254, 888   (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)

109.5   (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.86045 – 1707.26/(196.66 + t/°C)$; temp range 35–157°C (Antoine eq., Dean 1985, 1992)

110   (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.41271 – 1422.031/(t/°C + 165.444)$; temp range not specified (Riddick et al. 1986)

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

$\log (P_L/kPa) = 6.41271 – 1422.031/(–107.706 + T/K)$; temp range 325–431 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 10.60355 – 3986.406/(46.713 + T/K)$; temp range 298–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 53.9686 – 4.9501 \times 10^3/(T/K) – 15.199 \cdot \log(T/K) – 6.6922 \times 10^{-10} \cdot (T/K) + 2.3647 \times 10^{-6} \cdot (T/K)^2$; temp range 229–611 K (vapor pressure eq., Yaws 1994)

113*   (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)

$\ln (P/kPa) = 8.472727 – 1275.055/(T/K – 178.568)$; temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

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

1.562   (measured partial pressure/mole fraction x at dilute aqueous solution, Butler et al. 1935)

1.735   (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

1.562   (exptl., Hine & Mookerjee 1975)

1.88, 2.367 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.46   (limiting activity coefficient by headspace-GC., Abraham et al. 1987)

1.60   (calculated-MCI χ, Nirmalakhandan & Speece 1988b)

1.896   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

1.56   (limiting activity coefficient by headspace-GC., Li & Carr 1993)

1.016   (wetted-wall column-GC, Altschuh et al. 1999)

2.60   (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)

$\ln K_{AW} = 11.705 – 5538.7/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

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

2.03   (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Dunn III 1972)

1.99   (HPLC-RV correlation, Yonezawa & Urushigawa 1979)

2.03   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

1.86   (RP-HPLC-k' correlation, D'Amboise & Hanai 1982)

2.03   (HPLC-k' correlation, Funasaki et al. 1986)

2.04   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)

2.03   (generator column-GC, Schantz & Martire 1987)

2.05   (calculated from measured γ, Schantz & Martire 1987)

1.50   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

2.03   (recommended, Sangster 1989, 1993)

2.03   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.711   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

    1.01   (soil, quoted exptl., Meylan et al. 1992)

    0.92   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

    1.01   (calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

    Volatilization: evaporation rate of 1.85×10^{-5} mol·cm^{-2}·h^{-1} was determined by gravimetric method with an air flow rate of (50 ± 1) L·h^{-1} at (20 ± 0.1)°C (Gückel et al. 1973).

    Photolysis:

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

        photooxidation $t_{1/2} = 0.24$–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

        k_{OH}(exptl) $= (12.4 \pm 0.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) $= 10.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

        k_{OH}(exptl) $= 1.24 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K, and k(soln) $= 1.20 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction with OH radical in aqueous solution (Wallington et al. 1988b)

        $k_{OH} = 12.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1989)

        $k_{OH} = (12.2 \pm 2.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by pulse radiolysis-UV spectroscopy; $k_{OH} = (12.9 \pm 1.2) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

        k_{OH}(calc) $= 10.48 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

    Air: $t_{1/2} = 0.24$–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

    Surface water:

    Groundwater:

    Sediment:

    Soil:

    Biota

TABLE 11.1.1.10.1

Reported aqueous solubilities of 1-hexanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
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	7800	0	8100	5.51	7879	0	7900
10	6700	10	7000	6.85	7655	10	6900
20	5900	20	6400	8.15	7375	20	6200
30	5450	30	5900	11.0	7061	25	6000
40	5200	40	5400	12.94	6820	30	5700
50	5150	50	5000	14.68	6651	40	5300
60	5300	60	5200	17.04	6427	50	5100
70	5650	70	5600	20.71	6124	60	5200
80	6200	80	6100	22.99	5894	70	5600

(Continued)

TABLE 11.1.1.10.1 *(Continued)*

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
90	6800	90	6900	25.01	5838	80	6200
100	7850	100	8000	26.99	5764	90	6900
110	8900	110	9100	28.94	5702	100	7900
		120	10400	30.92	5639	110	9000
		130	11900	33.59	5560	120	10000
		140	13700			130	12000
		150	16300			140	14000
		160	20500			150	16000
		170	27000			160	21000
		180	36100			170	27000
		190	48700			180	36000
		200	67500			190	49000
		210	97000			200	68000
		220	163000			210	97000
						220	163000

2.

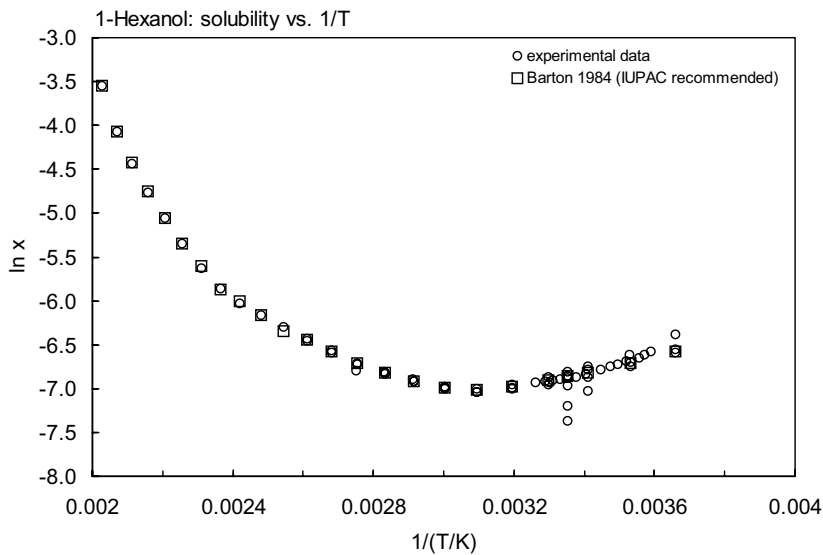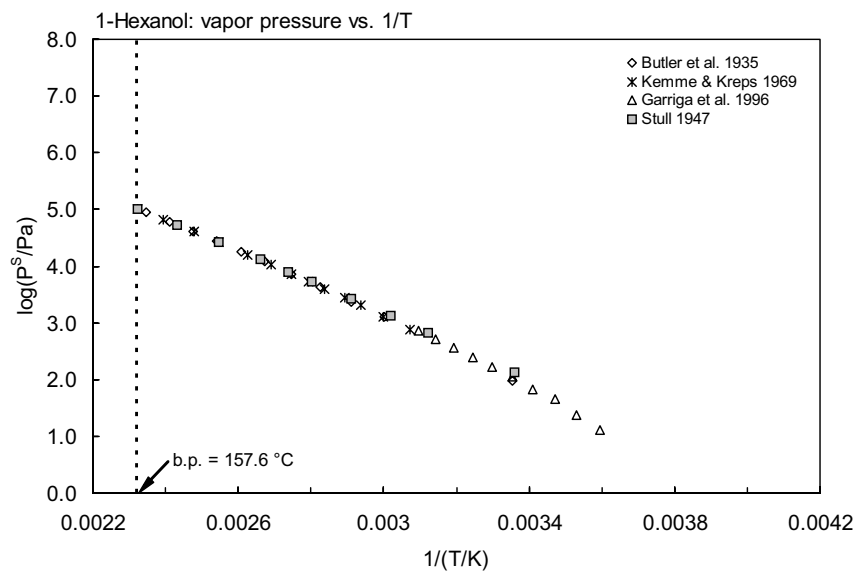| Stephenson et al. 1984	
shake flask-GC/TC	
t/°C	S/g·m⁻³
0	9640
10.2	7590
20.0	6660
29.7	5580
39.8	5140
50.0	4970
60.0	5180
70.3	5770
80.3	6250
90.3	6380

FIGURE 11.1.1.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-hexanol.

TABLE 11.1.1.10.2
Reported vapor pressures of 1-hexanol at various temperatures and the coefficients for the vapor pressure equations

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

Butler et al. 1935		Stull 1947		Kemme & Kreps 1969		Garriga et al. 1996	
static method-isteniscope		summary of literature data		differential thermal analysis		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	95.86	24.4	133.3	52.2	760.0	5	13
60.11	1300	47.2	666.6	60.4	1293	10	24
70.29	2365	58.2	1333	67.4	2040	15	45
80.58	4213	70.3	2666	72.6	2733	20	68
90.83	7275	83.7	5333	79.2	3973	25	113
101.16	12000	92.0	7999	85.0	5436	30	169
110.19	18012	102.8	13332	91.1	7373	35	251
120.55	27624	119.6	26664	98.7	10666	40	369
130.88	41303	138.0	53329	107.6	16105	45	517
141.67	60901	157.0	101325	119.7	26798	50	713
152.77	87966			130.1	40237		
		mp/°C	−51.6	144.5	66661	Antoine eq.	
bp/°C	155.7			157.3	100965	eq. 3a	P/kPa
D²⁵	0.8183					A	8.472727
				Antoine eq.		B	1275.055
eq. 4	P/mmHg			eq. 2	P/mmHg	C	−178.875
A	51.003			A	7.28781		
B	5068			B	1422.031		
C	13.80			C	165.444		

$\Delta H_V/(kJ\ mol^{-1}) = 62.84$
at 25°C

FIGURE 11.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexanol.

11.1.1.11 1-Heptanol

                                                              OH
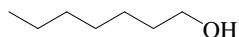
Common Name: 1-Heptanol
Synonym: 1-heptanol, *n*-heptyl alcohol
Chemical Name: *n*-heptyl alcohol, 1-heptanol
CAS Registry No: 111-70-6
Molecular Formula: $C_7H_{16}O$, $CH_3(CH_2)_6OH$
Molecular Weight: 116.201
Melting Point (°C):
  −33.2   (Lide 2003)
Boiling Point (°C):
  176.45   (Lide 2003)
Density (g/cm³ at 20°C):
  0.82053   (25°C, Butler et al. 1935)
  0.8219   (Weast 1982–83; Dean 1985)
Molar Volume (cm³/mol):
  142.0   (calculated-density, Lande & Banerjee 1981)
  170.2   (calculated- Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
  56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  930*   (18°C, shake flask-turbidity, measured range 70–130°C, Fühner 1924)
  1804   (shake flask-interferometer, Butler et al. 1933)
  1720   (20°C, shake flask-titration, Addison 1943)
  3288   (shake flask-centrifuge, Booth & Everson 1948)
  1200   (shake flask-turbidimetric method, Harkins & Oppenheimer 1949)
  2000*   (20°C, synthetic method, measured range 0–245°C, von Erichsen 1952)
  1800   (estimated, McGowan 1954)
  1700   (surface tension, Kinoshita et al. 1958)
  1500*   (20°C, surface tension, 15–60 °C, measured range Vochten & Petre 1973)
  1676*   (shake flask-interferometric method, measured range 6–34.9°C, Hill & White 1974)
  1313   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
  1740*   (recommended best value, IUPAC Solubility Data Series, temp range 0–240°C, Barton1984)
  1840*   (20.2°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson et al. 1984)
  1510   (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  29.86*   (extrapolated, modified isoteniscope method, measured range 60–110°C, Butler et al. 1935)
  log (P/mmHg) = 55.1972 – 5580/(T/K) – 15.41·log (T/K); temp range 60–152°C (isoteniscope measurements, Butler et al. 1935)
  44.04*   (extrapolated-regression of tabulated data, temp range 42.4–175.8°C, Stull 1947)
  22.2   (extrapolated-Antoine eq., ebulliometry, Kemme & Kreps 1969)
  626.6*   (63.5°C, ebulliometry-differential thermal analysis, measured range 63.6–176.4°C, Kemme & Kreps 1969)
  log (P/mmHg) = 6.85450 – 1266.783/(139.663 + t/°C); temp range 63.6–176.4°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
  31.30   (calculated-Antoine eq., Jordan 1970)
  log (P/mmHg) = [–0.2185 × 13920.9/(T/K)] + 9.720613; temp range 42.4–175.8°C (Antoine eq., Weast 1972–73)

12.8   (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

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

log (P/kPa) = 6.10824 – 1323.566/(146.241 + t/°C); temp range 63.6–176.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.01857 – 1278.78/(146.403 + t/°C); temp range 60.11–152.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

17.64   (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 6.64767 – 1140.64/(126.56 + t/°C); temp range 60–176°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 5.9794 – 1256.783/(–133.487 + T/K); temp range 336–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.10408 – 1322.62/(–126.87 + T/K); temp range 335–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/mmHg) = –19.9205 – 4.3239 × 10^3/(T/K) + 18.794·log (T/K) – 5.0553 × 10^{-2}·(T/K) + 2.6161 × 10^{-5}·(T/K)^2; temp range 239–632 K (vapor pressure eq., Yaws 1994)

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

1.909   (measured partial pressure/mole fraction *x* at dilute concn, Butler et al. 1935)

1.880   (exptl., Hine & Mookerjee 1975)

2.656, 3.583 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.015   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

1.176   (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

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

5.62   (gas stripping-GC, Shiu & Mackay 1997)

1.165   (wetted-wall column-GC, Altschuh et al. 1999)

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

2.53   (Hansch & Dunn III 1972)

2.41   (HPLC-RV correlation, Yonezawa & Urushigawa 1979)

2.57   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

2.39   (RP-HPLC-k' correlation, D'Amboise & Hanai 1982)

2.60   (HPLC-k' correlation, Funasaki et al. 1986)

2.65   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)

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

2.57   (generator column-GC, Schantz & Martire 1987)

2.57   (calculated-activity coeff. γ, Schantz & Martire 1987)

1.83   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

2.62   (recommended, Sangster 1989, 1993)

2.72   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

1.09   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

1.48   (calculated-MCI χ, Gerstl & Helling 1987)

1.14   (soil, quoted exptl., Meylan et al. 1992)

1.19   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.14   (soil, calculated-MCI ^{1}χ, Sabljic et al. 1995)

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

Volatilization: evaporation rate of 6.804 × 10^{-6} mol cm^{-2} h^{-1} was determined by gravimetric method with an air flow rate of (50 ± 1) L h^{-1} at 20°C (Gückel et al. 1973).

Photolysis:

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

photooxidation $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical in air (Darnall et al. 1976)

k_{OH}(exptl) = (13.6 ± 1.3) × 10^{-12} cm^{-1} $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 10.5 × 10^{-12} cm^{-1} $molecule^{-1}$ s^{-1} at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

k_{OH}(exptl) = 1.36 × 10^{-12} cm^{-1} $molecule^{-1}$ s^{-1}, and k(soln) = 1.20 × 10^{-11} cm^{-1} $molecule^{-1}$ s^{-1} for the s reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH} = (13.7 ± 1.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K (relative rate method, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical in air (Darnall et al. 1976).

Surface water:

Sediment:

Soil:

Biota:

TABLE 11.1.1.11.1
Reported aqueous solubilities of 1-heptanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
70	1250	0	3400	15	2000	6.0	2204
80	1700	10	2600	20	1500	10.2	2020
90	2250	20	2000	30	1500	10.54	1998
100	2800	30	1600	40	1300	15.08	1868
110	3350	40	1300	50	1400	17.94	1794
120	4300	50	1100	60	1500	20.03	1750
130	5150	60	1100			21.9	1685
		70	1500			24.99	1676
		80	1900			25.07	1665
		90	2300			26.04	1652
		100	2900			28.02	1639
		110	3500			30.14	1623
		120	4300			30.16	1625
		130	5300			32.9	1610
		140	6500			34.9	1605
		150	8000				
		160	9800				
		170	12300				
		180	16000				
		190	20800				
		200	25400				
		210	34800				

TABLE 11.1.1.11.1 *(Continued)*

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
		220	46800				
		230	67000				
		240	101000				
		245	139600				

2.

| Barton 1984				Stephenson et al. 1984	
IUPAC recommended				shake flask-GC/TC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
0	3400	120	4300	0	2360
10	2500	130	5200	10.5	2530
20	1700	140	6500	20.2	1840
25	1740	150	8000	30.6	1540
30	1600	160	10000	39.8	1660
40	1300	170	12000	50.1	1620
50	1200	180	16000	60.0	1780
60	1300	190	21000	70.1	2040
70	1400	200	26000	80.1	2170
80	1800	210	35000	90.5	2430
90	2300	220	47000		
100	2900	230	67000		
110	3400	240	101000		
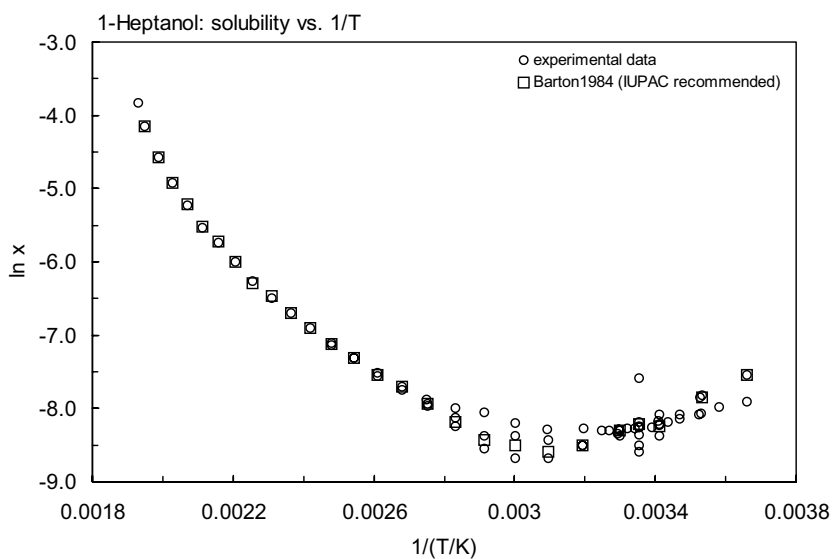
FIGURE 11.1.1.11.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1-heptanol.

TABLE 11.1.1.11.2

Reported vapor pressures of 1-heptanol 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)	

Butler et al. 1935		Stull 1947		Kemme & Kreps 1969	
isoteniscope method		summary of literature data		differential thermal analysis	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	29.86	42.4	133.3	63.6	626.6
68.11	505	64.3	666.6	76.1	1453
70.29	997	74.7	1333	81.5	2000
80.58	1913	85.8	2666	87.6	2813
90.83	3430	99.8	5333	94.3	4026
101.16	5882	108.0	7999	99.9	5360
110.10	9061	119.5	13332	106.4	7399
120.55	14292	136.6	26664	114.5	10732
130.88	21811	155.6	53329	124.1	16319
141.67	32864	175.8	101325	136.5	26798
152.77	48596			147.8	40463
		mp/°C	34.6	162.8	66794
bp/°C	175.6			178.4	101432
D^{25}	0.8205				
				Antoine eq.	
eq. 4	P/mmHg			eq. 2	P/mmHg
A	56.1972			A	6.85450
B	5580			B	1256.783
C	15.41			C	139.663

$\Delta H_V/(kJ\ mol^{-1}) = 68.66$
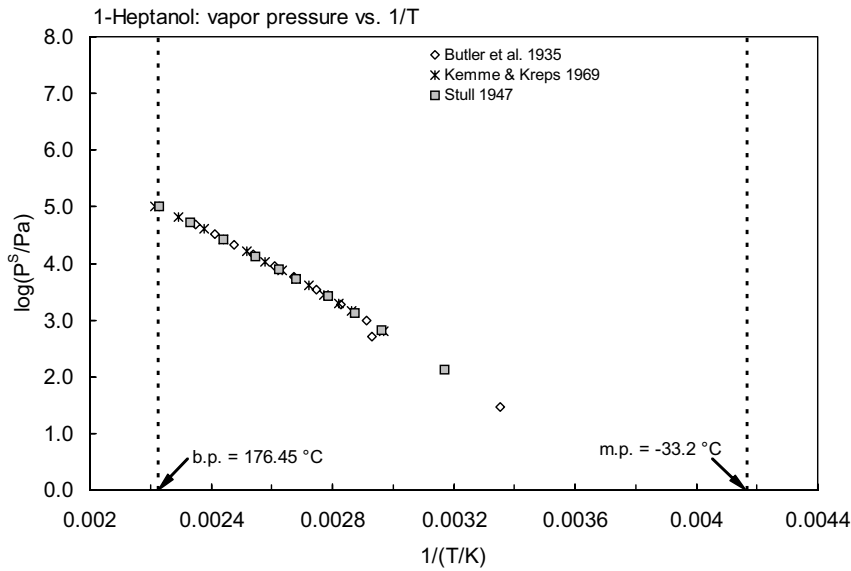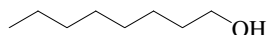at 25°C

FIGURE 11.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1-heptanol.

11.1.1.12 1-Octanol (*n*-Octyl alcohol)

Common Name: 1-Octanol
Synonym: 1-octanol, *n*-octyl alcohol, capryl alcohol, heptylcarbinol
Chemical Name: *n*-octyl alcohol, 1-octanol
CAS Registry No: 111-87-5
Molecular Formula: $C_8H_{18}O$, $CH_3(CH_2)_7OH$
Molecular Weight: 130.228
Melting Point (°C):
    –14.8   (Lide 2003)
Boiling Point (°C):
    195.15   (Lide 2003)
Density (g/cm³ at 20°C):
    0.827   (Weast 1982–83)
    0.82499, 0.82157   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    158.0   (calculated-density, Rohrschneider 1973; Lande & Banerjee 1981)
    192.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    42.3   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    56   (estimated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    586   (shake flask-interferometer, Butler et al. 1933)
    760   (30°C, shake flask-titration, Sobotka & Glick 1934.)
    420   (20°C, shake flask-surface tension, Addison 1945)
    590   (shake flask-turbidimeter, McBain & Richard 1946)
    500   (shake flask-titration, Crittenden & Hixon 1954)
    582   (estimated, McGowan 1954)
    490   (shake flask-surface tension, Kinoshita et al. 1958)
    495   (shake flask-turbidity, Shinoda et al. 1959)
    1000   (30°C, shake flask-turbidimeter, Rao et al. 1961)
    330   (calculated-K_{OW}, Hansch et al. 1968)
    530   (15°C, shake flask-surface tension, Vochten & Petre 1973)
    600, 600   (40, 60°C, shake flask-titration, Lavrova & Lesteva 1976)
    10000, 5000 (95, 115°C, shake flask-polythermic method, Zhuravleva et al. 1977)
    540*   (recommended best value, IUPAC Solubility Data Series, temp range 15–115°C, Barton 1984)
    490*   (20.5°C, shake flask-GC/TC, measured range 20.5–90.3°C, Stephenson et al. 1984)
    517   (shake flask-GC, Li et al. 1992)
    417   (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    11.06*   (25°C, extrapolated-modified isoteniscope data, measured range 60.12–110°C, Butler et al. 1935)
    log (P/mmHg) = 40.2105 – 4100/(T/K) – 10.35·log (T/K); temp range 20–110°C (isoteniscope measurements,
        Butler et al. 1935)
    18.8*   (extrapolated-regression of tabulated data, temp range 54–195.2°C, Stull 1947)
    log (P/mmHg) = 8.29442 – 2302.3/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    7604*   (121.99°C, ebulliometry, measured range 121.99–195.28°C, Dreisbach & Shrader 1949)

5.28 (extrapolated-Antoine eq., ebulliometry- DTA, Kemme & Kreps 1969)

706.6* (78.9°C, ebulliometry-differential thermal analysis, measured range 78.9–195.3°C, Kemme & Kreps 1969)

log (P/mmHg) = 6.62354 – 1196.639/(124.107 + t/°C); temp range 78.9–195.3°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

10* (comparative ebulliometry, measured range 113.274–206.123 K, Ambrose & Sprake 1970)

log (P/Pa) = 5.79413 – 1434.755/(T/K – 149.407); restricted temp range 113.274–151.974°C, (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 5.88511 – 1264.322/(T/K – 142.420); temp range 113.274–206.123°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

142* (54.88°C, comparative ebulliometry, measured range 328.03–386.96 K, data fitted to Chebyshev polynomial, Ambrose et al. 1974)

2.78 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)

4.07, 32.3, 177 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)

log (P/mmHg) = [–0.2185 × 14262.4/(T/K)] + 9.601156; temp range: 54–195°C, (Antoine eq., Weast 1972–73)

10.06, 6.89, 5.74. 9.95 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.80512 – 1752.302/(174.07 + t/°C); temp range 54.88–113.9°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)

log (P/kPa) = 5.98227 – 1322.952/(137.413 + t/°C); temp range 79.9–195.4°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

log (P/kPa) = 5.87970 – 1260.554/(130.23 + t/°C); temp range 113.3–206.1°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 6.00162 – 1356.232/(144.452 + t/°C); temp range 229.05–250.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

13.43 (calculated-Antoine eq., Dean 1985)

log (P/mmHg) = 12.0701 – 4506.8/(319.9 + t/°C); temp range 0–80°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.83790 – 1310.62/(136.05 + t/°C); temp range 70–195°C (Antoine eq., Dean 1985, 1992)

14.5 (static measurement, Berti et al. 1986)

10.0 (Riddick et al. 1986)

log (P/kPa) = 5.88511 – 1264.322/(t/°C + 130.73); temp range not specified (Riddick et al. 1986)

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

log $(P_L$/kPa) = 5.90052 – 1273.291/(–141.417 + T/K); temp range 386–480 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 5.342 – 3343/(T/K); temp range 267–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 18.014 – 5507/(T/K); temp range 238–251 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 5.7934 – 1208.201/(–149.366 + T/K); temp range 430–474 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 6.39406 – 1540.599/(–114.618 + T/K); temp range 328–400 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 5.90632 – 1276.86/(–140.996 + T/K); temp range 397–479 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

10.58 (Daubert & Danner 1989; quoted, Howard 1993)

log (P/mmHg) = –26.3876 – 4.2263 × 10^3/(T/K) + 21.093·log(T/K) – 5.0048 × 10^{-2}·(T/K) + 2.4611 × 10^{-5}·(T/K)^2; temp range 258–653 K (vapor pressure eq., Yaws 1994)

8.0* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)

ln (P/kPa) = 13.058110 – 2443.493/(T/K – 162.071); temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

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

2.454 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)

2.479 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

2.422 (exptl., Hine & Mookerjee 1975)

3.344, 6.085 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.537 (calculated-MCI χ, Nirmalakhandan & Speece 1988)

1.609   (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1.537   (wetted-wall column-GC, Altschuh et al. 1999)

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

3.15   (shake flask-CR, Collander 1951)
2.84   (calculated-π constant, Hansch et al. 1968)
3.03   (Hansch & Dunn III 1972)
2.95, 2.97; 2.84   (calculated-f const.; calculated-π constant, Rekker 1977)
2.97   (HPLC-k' correlation, Könemann et al. 1979)
2.80   (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
2.92   (RP-HPLC-k' correlation, D'Amboise & Hanai 1982)
3.16   (shake flask-GC, Platford 1983)
2.97   (Hansch & Leo 1985)
3.27   (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
2.14   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
3.07   (recommended, Sangster 1989, 1993)
3.00   (recommended, Hansch et al. 1995)

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

6.03   (calculated-measured γ° in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

0.307   (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)
0.097   (calculated-S, Lyman et al. 1982; quoted, Howard 1993)
1.651   (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

2.99   (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)
2.14   (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
1.56, 1.76   (quoted, calculated-MCI χ, Gerstl & Helling 1987)
1.56   (soil, quoted exptl., Meylan et al. 1992)
1.45   (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.56   (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization: evaporation rate k = 1.752×10^{-6} mol·cm^{-2}·h^{-1} was determined by gravimetric method with an air
    flow rate k = (50 ± 1) L h^{-1} at $20 \pm 0.1°C$ (Gückel et al. 1973);
    $t_{1/2}$ ~1.8 d from a model river of 1-m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated
        Henry's law constant (Lyman et al. 1982; quoted, Howard 1993);
    $t_{1/2}$ ~8.2 d from a model pond with the consideration of adsorption (USEPA 1987; quoted, Howard 1993).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
    with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures see reference:
    photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate
        of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
    k ≤ 0.8 M^{-1} s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)
    k_{OH} = $(13.6 \pm 1.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Wallington et al. 1988a; Atkinson 1989)
    k_{OH} = $(14.4 \pm 1.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Nelson et al. 1990)
    k_{OH}(calc) = 11.67×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

    Air: $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance
        of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

        photooxidation $t_{1/2}$ = 1.3 d in air, based on measured rate constant k = 1.195 × 10^{-11} cm^3 molecule^{-1} s^{-1} for
            the vapor-phase reaction with photochemically produced hydroxyl radical of 5 × 10^5 cm^{-3} at 25°C in air
            (Atkinson 1987; quoted, Howard 1993).

    Surface water:
    Groundwater:
    Sediment:
    Soil:
    Biota:

TABLE 11.1.1.12.1
Reported aqueous solubilities of 1-octanol at various temperatures

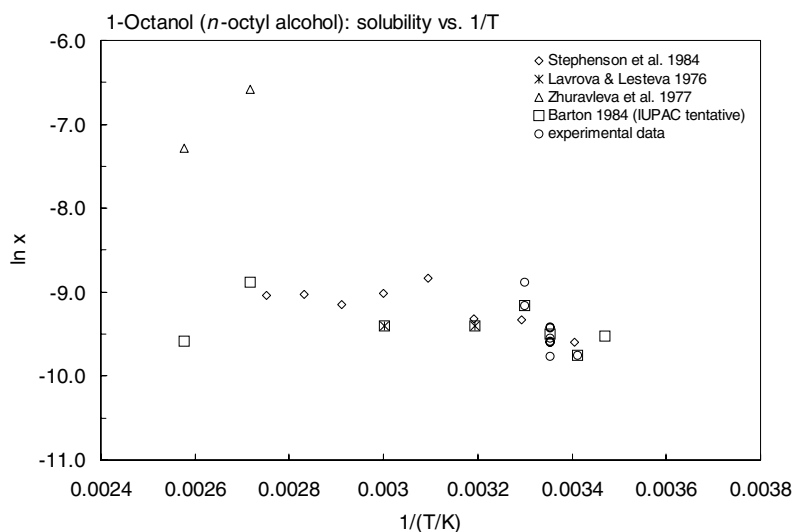| Barton 1984		Stephenson et al. 1984	
tentative or recommended		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	530	20.5	490
20	420	30.6	640
25	540	40.1	650
30	760	50.0	1050
40	600	60.3	880
60	600	70.3	770
95	1000	80.1	870
115	500	90.3	860
25	540*		
30	900*		

*"best" values

FIGURE 11.1.1.12.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-octanol.

TABLE 11.1.1.12.2
Reported vapor pressures of 1-octanol at various temperatures and the coefficients for the vapor pressure equations

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

1.

Butler et al. 1935		Stull 1947		Dreisbach & Shrader 1949		Kemme & Kreps 1969	
isoteniscope method		summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	11.066	54.0	133.3	121.99	7604	78.9	706.6
60.12	220.0	76.5	666.6	125.42	8851	88.8	1360
70.3	441.3	88.3	1333	140.37	16500	95.4	2000
80.59	890.6	101.0	2666	166.09	42066	101.5	2800
90.84	1589	115.2	5333	181.17	67661	108.4	4000
101.17	2868	123.8	7999	195.28	101325	114.0	5266
110.2	4456	135.2	13332			120.9	7253
120.56	7202	152.0	26664			131.2	11386
130.89	11390	173.8	53329			140.2	16505
141.68	17683	195.2	101325			166.1	42063
152.78	26858					181.2	67674
		mp/°C	−15.4			195.3	101325
bp/°C	194.5						
D^{25}	0.8232					Antoine eq.	
						eq. 2	P/mmHg
eq. 4	P/mmHg					A	6.62354
A	65.2106					B	1196.639
B	6190					C	124.107
C	18.40						
$\Delta H_V/(kJ \; mol^{-1}) = 72.93$							
at 25°C							

2.

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
113.274	5065	54.88	142	5	< 2
117.718	6261	64.11	281	10	< 2
122.526	7810	70.44	431	15	< 2
127.503	9742	73.91	544	20	3
133.164	12400	77.69	700	25	8
139.162	15845	79.86	803	30	15
147.224	21679	82.36	938	35	25
151.974	25859	84.65	1078	40	45
157.372	31373	87.26	1259	45	77
161.868	36654	89.24	1415	50	116
167.897	44832	91.26	1591		
173.981	54475	95.52	2022	Antoine eq.	

TABLE 11.1.1.12.2 (*Continued*)

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
179.523	64637	101.66	2817	eq. 3a	P/Pa
184.300	74519	105.12	5376	A	13.058110
190.026	87866	109.57	4226	B	2443.493
195.114	101222	113.81	5236	C	−162.071
195.504	102265				
201.198	119164	data fitted to Chebyshev			
206.123	135431	polynomial, see ref.			

Antoine eq. for full range

eq. 3	P/Pa
A	5.88511
B	1264.322
C	−142.420

Data also fitted to Cragoe
equation, see ref.
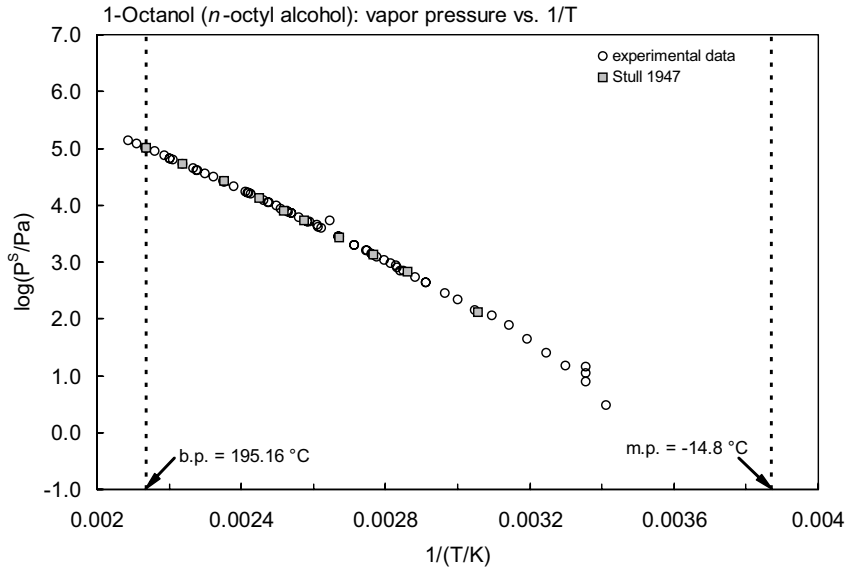
FIGURE 11.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for 1-octanol.

11.1.1.13 1-Nonanol
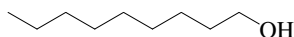
Common Name: 1-Nonanol
Synonym: *n*-nonyl alcohol
Chemical Name: 1-nonanol
CAS Registry No: 143-08-8
Molecular Formula: $C_9H_{20}O$, $CH_3(CH_2)_8OH$
Molecular Weight: 144.254
Melting Point (°C):
     –5   (Lide 2003)
Boiling Point (°C):
     213.37   (Lide 2003)
Density (g/cm³ at 20°C):
     0.8273   (Weast 1982–83)
Molar Volume (cm³/mol):
     174.4   (20°C, Stephenson and Malanowski 1987)
     214.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, 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/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
     compiled at the end of this section):
     140   (shake flask-surface tension, Kinoshita et al. 1958)
     140   (15°C, shake flask-surface tension, Vochten and Petre 1973)
     130   (recommended-IUPAC Solubility Data Series, Barton 1984)
     280*   (20°C, shake flask-GC/TC, measured range 9.8–90.5°C, Stephenson & Stuart 1986)
     128   (20°C, shake flask/slow stirring-GC, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at
     other temperatures designated * are compiled at the end of this section):
     133.3*   (59.5°C, summary of literature data, temp range 59.5–213.5°C, Stull 1947)
     746.6*   (91.7°C, ebulliometry-differential thermal analysis, measured range 91.7–213.6°C, Kemme & Kreps
               1969)
     log (P/mmHg) = 6.83667 – 1373.417/(133.968 + t/°C); temp range 91.7–213.6°C, or pressure range 5.6–757.5
               mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
     log (P/mmHg) = [–0.2185 × 14065.1/(T/K)] + 8.99150; temp range 69.5–231°C (Antoine eq., Weast 1972–73)
     7.466   (20°C, extrapolated from data of Stull 1947, Gückel et al. 1973)
     1.87   (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
     12680*   (152.15°C, ebulliometry, measured range 152–221.35°C, Hon et al. 1976)
     0.106   (20°C, evaporation rate-gravimetric method, Gückel et al. 1982)
     log (P_L/kPa) = 5.9049 – 1341.28/(–142.64 + T/K); temp range 381–495 K (Antoine eq.-I, Stephenson &
               Malanowski 1987)
     log (P_L/kPa) = 5.9454 – 1366.566/(–139.73 + T/K); temp range 368–500 K (Antoine eq.-II, Stephenson &
               Malanowski 1987)
     log (P/mmHg) = 103.0308 –8.1526 × 10³/(T/K) –31.641·log(T/K) – 7.230 × 10⁻¹⁰·(T/K) + 6.0332 × 10⁻⁶·(T/K)²;
               temp range 280–690 K (vapor pressure eq., Yaws 1994)

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

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

3.77	(generator column-GC, Tewari et al. 1982)
4.26	(shake flask, Log P Database, Hansch & Leo 1987)
4.26	(recommended, Sangster 1993)
4.26	(shake flask, recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

TABLE 11.1.1.13.1
Reported aqueous solubilities of 1-nonanol at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	$S/g \cdot m^{-3}$
9.8	350
20.0	280
29.6	310
39.6	340
49.8	320
60.1	340
70.5	330
80.2	280
90.5	300
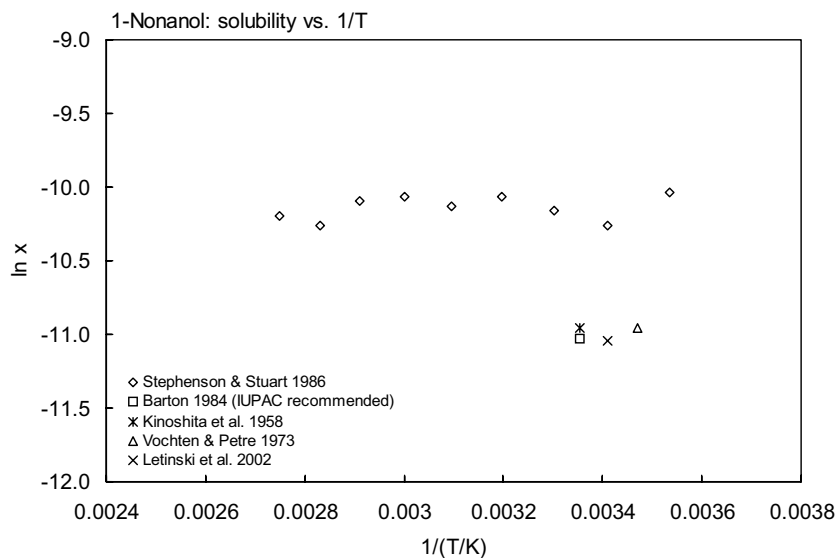
FIGURE 11.1.1.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-nonanol.

TABLE 11.1.1.13.2
Reported vapor pressures of 1-nonanol 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)		

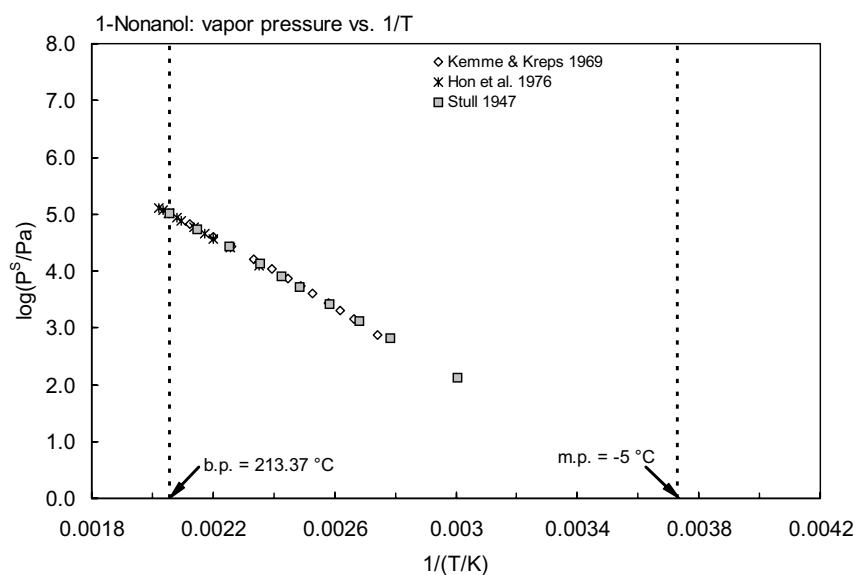| Stull 1947		Kemme & Kreps 1969		Hon et al. 1976	
summary of literature data		differential thermal analysis		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		ebulliometry			
59.5	133.1	91.7	746.6	152.15	12680
86.1	666.6	102.1	1400	170.20	25385
99.7	1333	108.9	2040	181.03	37146
113.8	2666	114.4	2706	187.49	46110
129.0	5333	122.4	4026	194.80	58337
139.0	7999	128.8	5413	203.95	77352
151.3	13332	135.8	7399	207.76	86645
170.5	26664	144.7	10719	213.44	101948
192.1	53329	155.0	16092	213.97	103527
213.5	101325	169.0	26851	217.73	115289
		181.0	40317	221.35	127515
mp/°C	−5	198.0	66994		
		213.6	101845	bp/°C	213.17
		Antoine eq.		eq. 2	P/mmHg
		eq. 2	P/mmHg	A	7.60022
		A	6.83667	B	1793.77
		B	1373.417	C	166.91
		C	133.968		

FIGURE 11.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 1-nonanol.

11.1.1.14 1-Decanol
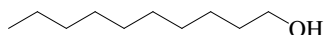
Common Name: 1-Decanol
Synonym: decyl alcohol
Chemical Name: 1-decanol
CAS Registry No: 112-30-1
Molecular Formula: $C_{10}H_{22}O$, $CH_3(CH_2)_8CH_2OH$
Molecular Weight: 158.281
Melting Point (°C):
  6.9   (Lide 2003)
Boiling Point (°C):
  231.1   (Lide 2003)
Density (g/cm³ at 20°C):
  0.8297   (Weast 1982–83)
Molar Volume (cm³/mol):
  190.8   (20°C, calculated-density, Stephenson and Malanowski 1987)
  236.8   (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: 1.0

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

  50   (shake flask-turbidimetric method, Stearns et al. 1947)
  36   (20°C, shake flask-surface tension, Addison and Hutchinson 1949)
  50   (shake flask-turbidimetric method-photometer, Harkins and Oppenheimer 1949)
  37   (shake flask-surface tension, Kinoshita et al. 1958)
  32   (15°C, shake flask-surface tension, Vochten and Petre 1973)
  10000, 8000   (102.5, 120.5°C, polythermic method, Zhuravleva et al. 1977)
  37*   (recommended-IUPAC Solubility Data Series, temp range 15–120°C, Barton 1984)
  210*   (29.6°C, shake flask-GC/TC, measured range 29.6–90.4°C, Stephenson 1992)
  35.9   (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
   temperatures designated * are compiled at the end of this section):
  133.3*   (69.5°C, summary of literature data, temp range 69.5–231.0°C, Stull 1947)
  747*   (105.0°C, ebulliometry-differential thermal analysis, measured range 105–231°C, Kemme & Kreps
               1969)
  log (P/mmHg) = 6.39379 – 1180.306/(104.321 + t/°C); temp range 105–231°C, or pressure range 5.6–757.5
       mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
  1.0*   (comparative ebulliometry, measured range 127.261–255.2°C, Ambrose & Sprake 1970)
  log (P/Pa) = 5.94387 – 1434.755/(T/K – 139.888); restricted temp range 127.261–194.484°C (Antoine eq., com-
       parative ebulliometry, Ambrose & Sprake 1970)
  log (P/Pa) = 5.86571 – 1373.916/(T/K – 147.202); temp range 127.16–255.2°C (Antoine eq., comparative ebul-
       liometry, Ambrose & Sprake 1970)
  124*   (76.23°C, comparative ebulliometry, measured range 349.38–406.19 K, data fitted to Chebyshev
               polynomial, Ambrose et al. 1974)
  log (P/mmHg) = [–0.2185 × 13849.2/(T/K)] + 9.115470; temp range 59.5–213.5°C (Antoine eq., Weast 1972–73)
  0.5866   (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
  1.10   (20°C, evaporation rate-gravimetric method, Gückel 1982)

log (P/kPa) = 5.76028 – 1315.079/(119.128 + t/°C), temp range 105–231°C (Antoine eq. derived from.exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

log (P/kPa) = 5.84611 – 1365.892/(124.619 + t/°C), temp range 127.2–255.2°C (Antoine eq. derived from data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P_S/kPa) = 17.615 – 6028/(T/K); temp range 264–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.57397 – 1761.308/(–113.992 + T/K); temp range 349–410 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.8587 – 1374.347/(–147.547 + T/K); temp range 405–528 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 111.7949 –8.3502 × 10³/(T/K) –34.786·log(T/K) + 3.3682 × 10⁻¹⁰·(T/K) + 7.2697 × 10⁻⁶·(T/K)²; temp range 268–673 K (vapor pressure eq., Yaws 1994)

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

  2.689   (computer value, Yaws et al. 1991)
  3.222   (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_OW:

  3.98   (HPLC-RT correlation, D'Amboise & Hani 1982)
  4.57   (shake flask, Log P Database, Hansch & Leo 1987)
  4.57   (recommended, Sangster 1993)
  4.57   (shake flask, recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_OA:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_OC:

Environmental Fate Rate Constant, k and Half-Lives, t_½:

Half-Lives in the Environment:

TABLE 11.1.1.14.1
Reported aqueous solubilities of 1-decanol at various temperatures

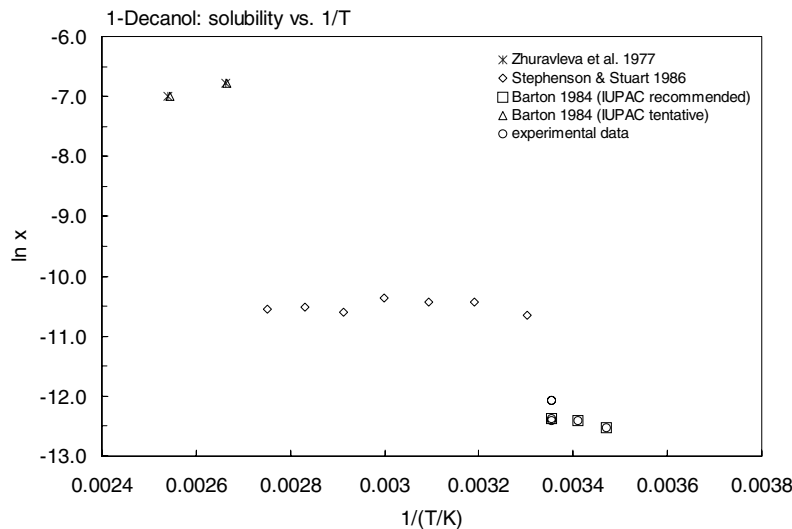| Barton 1984 | | Stephenson & Stuart 1986 | |
| IUPAC recommended | | shake flask-GC/TC | |
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
15	32	29.6	210
20	36	40.3	260
25	37	50.0	260
102	10000#	60.3	280
120	8000#	70.2	220
	# tentative	80.2	240
		90.4	230
		mp/°C	5

FIGURE 11.1.1.14.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-decanol.

TABLE 11.1.1.14.2
Reported vapor pressures of 1-decanol 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		Kemme & Kreps 1969		Ambrose & Sprake 1970		Ambrose & Sprake 1974	
summary of literature data		differential thermal analysis		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
69.5	133.3	105.0	747	127.261	2656	349.38	124
97.3	666.6	114.5	1360	129.526	2968	358.67	235
111.3	1333	121.7	2000	133.573	3600	364.21	339
125.8	2666	127.3	2680	138.245	4468	364.26	352
142.1	5333	135.6	3986	141.817	5242	371.15	528
152.9	7999	142.2	5346	147.863	6250	371.30	534
165.8	13332	149.9	7466	149.414	7266	375.86	701
186.2	26664	159.2	10812	154.602	8995	379.24	854
208.6	53329	169.9	16172	159.206	10799	380.38	917
231.0	101325	183.9	25398	163.693	12835	383.04	1061
		197.4	40397	168.653	15439	385.72	1236
mp/°C	7.0	215.3	67301	174.653	19146	388.16	1408
		231.0	101005	177.568	21193	392.43	1769
				182.748	25250	395.02	2025
		Antoine eq		189.377	31359	397.42	2283
		eq. 2	P/mmHg	194.484	36807	401.34	2774
		A	6.39397	201.039	44875	403.08	3017

(Continued)

TABLE 11.1.1.14.2 *(Continued)*

| Stull 1947 summary of literature data		Kemme & Kreps 1969 differential thermal analysis		Ambrose & Sprake 1970 comparative ebulliometry		Ambrose & Sprake 1974 comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1180.306	207.352	55899	404.70	3263
		C	104.321	213.119	63364	406.19	3504
				218.923	74244		
				225.489	87994		
				230.471	99886		
				237.598	118863		
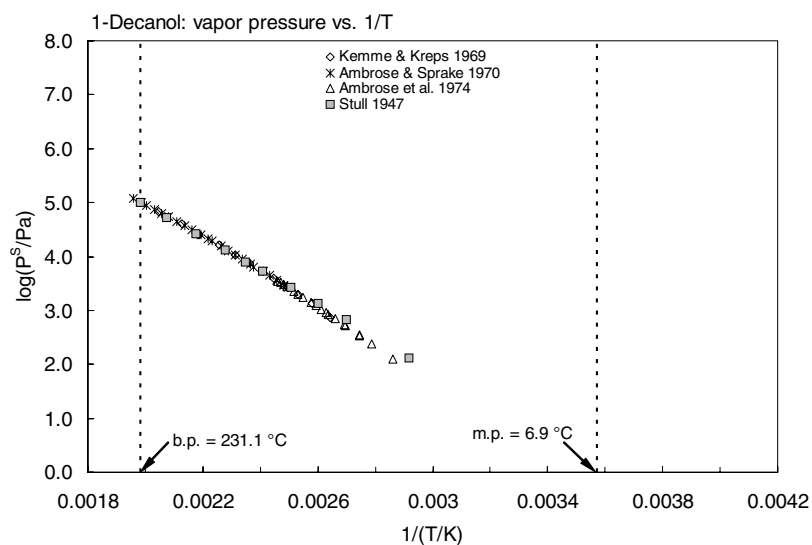
FIGURE 11.1.1.14.2 Logarithm of vapor pressure versus reciprocal temperature for 1-decanol.

11.1.1.15 Ethylene glycol

HO⌒OH
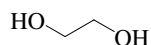
Common Name: Ethylene glycol
Synonym: 1,2-ethanediol, 1,2-dihydroxyethane, MEG
Chemical Name: 1,2-ethanediol, ethylene glycol
CAS Registry No: 107-21-1
Molecular Formula: $C_2H_6O_2$, $HOCH_2CH_2OH$
Molecular Weight: 62.068
Melting Point (°C):
    –12.69   (Lide 2003)
Boiling Point (°C):
    197.3   (Lide 2003)
Density (g/cm^3 at 20°C):
    1.1088   (Weast 1982–83)
Molar Volume (cm^3/mol):
    55.8   (Rohrschneider 1973)
    66.6   (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
    14.22   (Dean 1985)
    14.24   (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.958   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    miscible (Dean 1985; Howard 1990; Yaws et al. 1990)
    miscible (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    22.39   (extrapolated-Antoine eq., differential manometer, Gallaugher & Hibbert 1937)
    log (P/mmHg) = 9.2087 – 2976.6/(T/K); temp range 40–120°C (Antoine eq. from differential Hg manometry measurements, Gallaugher & Hibbert 1937)
    133.3*   (53.0°C, summary of literature data, temp range 53.0–197.3°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 14032.4/(T/K)] + 9.394685; temp range: 53–197.3°C (Antoine eq., Weast 1972–73)
    11.70*   (ebulliometry, extrapolated-Antoine eq., measured range 270–310 K, Ambrose & Hall 1981)
    log (P/kPa) = 11.1828 – 2611.2/[(T/K) – 40.0]; temp range 270–310 K (ebulliometry, Antoine eq., Ambrose & Hall 1981)
    log (P/kPa) = 6.83995 – 1818.591/[(T/K) – 94.499]; temp range 374.01–495.4 K (Antoine eq., ebulliometry, Ambrose & Hall 1981)
    7.40*   (20°C, average, gas saturation-GC/FID, Hales et al. 1981)
    log (P/mmHg) = 23.7259 – 4648.55/(T/K) – 503391/(T/K)$^{-2}$; temp range 283–373 K (empirical vapor pressure eq., gas saturation, Hales et al. 1981)
    14.90   (20°C, evaporation method, Gückel et al. 1982)
    6.67, 26.66   (20°C, 30°C, Verschueren 1983)
    0.73, 9.30   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.69339 – 1093.154/(98.821 + t/°C); temp range 122.5–186.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    log (P/kPa) = 7.13856 – 2035.185/(1936.936 + t/°C); temp range 50–200°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    11.86   (extrapolated-Antoine eq., Dean 1985)
    11.7   (Riddick et al. 1986)

log (P/kPa) = 6.83995 – 1818.591/(178.651 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 8.3726 – 2994.4/(T/K), temp range 130–190°C, (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 8.0908 – 2088.9/(203.5 + t/°C); temp range 50–200°C (Antoine eq., Dean 1985, 1992)

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

log (P$_L$/kPa) = 6.98465 – 1928.08/(–83.45 + T/K); temp range 323–473 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.86912 – 1817.439/(–95.859 + T/K), temp range 363–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)

12.26   (Howard et al. 1986; quoted, Banerjee et al. 1990)

log (P/mmHg) = 82.4062 – 6.3472 × 10^3/(T/K) – 25.433·log(T/K) – 2.3732 × 10^{-9}·(T/K) + 8.7467 × 10^{-6}·(T/K)^2; temp range 160–645 K (vapor pressure eq., Yaws 1994)

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

0.006   (calculated-C_W/C_A, Hine & Mookerjee 1975)

5.81 × 10^{-6}, 2.37 × 10^{-5} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K$_{OW}$:

–1.93   (shake flask, Hansch & Leo 1979)

–1.34   (shake flask-RC, Cornford 1982)

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

–1.36   (recommended, Sangster 1993)

–1.36   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

1.00   (golden ide, after 3 d, Freitag et al. 1985)

2.28   (algae, after 1 d, Freitag et al. 1985)

2.30   (activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, log K$_{OC}$:

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

Volatilization: evaporation rate k = 2.915 × 10^{-6} mol cm^{-2} h^{-1} was determined by gravimetric method with an air flow rate k = (50 ± 1) L h^{-1} at 20 ± 0.1°C (Gückel et al. 1973);

evaporation rate k = 2.97 × 10^{-8} mol cm^{-2} h^{-1} was determined at 20°C (Gückel et al. 1982).

Photolysis:

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

photooxidation t$_{1/2}$ = 267 d-64.6 yr in water, based on measured rate constant for the reaction with OH radical (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation t$_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

k$_{OH}$ = (7.7 ± 1.1) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 K in air (Wiedermann & Zetzsch 1982; quoted, Atkinson 1985)

photooxidation t$_{1/2}$ = 8.3–83 h in air, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

Hydrolysis:

Biodegradation:

k = 41.7 mg COD g^{-1} h^{-1}, average rate based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

k = 0.026–0.035 h^{-1} in 30 mg/L activated sludge after a time lag of 10–15 h (Urano & Kato 1986b)

t$_{1/2}$(aq. aerobic) = 48–288 h, based on grab sample from river die-away studies (Evans & David 1974; selected, Howard et al. 1991);

t$_{1/2}$(aq. anaerobic) = 192–1152 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:

Half-Lives in the Environment:

Air: t$_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
photooxidation t$_{1/2}$ = 8.3–83 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).
Surface water: photooxidation t$_{1/2}$ = 267 d-64.6 yr, based on measured rate constant for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991); t$_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Groundwater: t$_{1/2}$ = 96–576 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: t$_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota

TABLE 11.1.1.15.1

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

$\log P = A - B/(T/K)$ (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)		
$\log P = A - B/(T/K) - C/(T/K)^2$ (5)		$\ln P = A - B/(T/K) - C/(T/K)^2$ (5a)

1.

Stull 1947		Ambrose & Hall 1981		Hales et al. 1981			
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				"continuous" measurements		"collection" measurements	
53.0	133.3	100.86	2208	10.0	2.698	9.0	2.711
79.7	666.6	103.869	2584	9.68	2.834	9.8	2.706
92.1	1333	107.59	3121	8.97	2.656	9.79	2.938
105.8	2666	111.997	3885	10.01	7.285	10.02	2.873
120.2	5333	115.971	4705	19.91	7.565	9.73	2.825
129.5	7999	120.647	5857	20.05	7.174	9.94	2.805
141.8	13332	124.645	7032	39.85	14.94	10.09	2.795
158.5	26664	129.735	8800	39.97	43.54	19.9	7.254
178.5	53329	133.244	10244	39.77	42.48	19.05	7.084
197.3	101325	182.095	62918	59.72	44.12	19.93	7.577
		187.372	74338	59.94	184.9	20.51	7.911
mp/°C	–15.6	192.976	88398	60.04	187.8	19.93	7.495
		197.704	101829	59.72	197.8	20.0	7.210
		203.13	119270	74.55	466.2	20.0	7.710
		207.615	135464	74.57	476.9	39.97	41.84
		212.932	156959	73.74	472.6		
		217.989	179863	100.17	2166.0		
		222.287	201399	100.15	2098.0	overall best fit equation	
		25.0	11.70			eq. 5a	P/Pa

(Continued)

TABLE 11.1.1.15.1 *(Continued)*

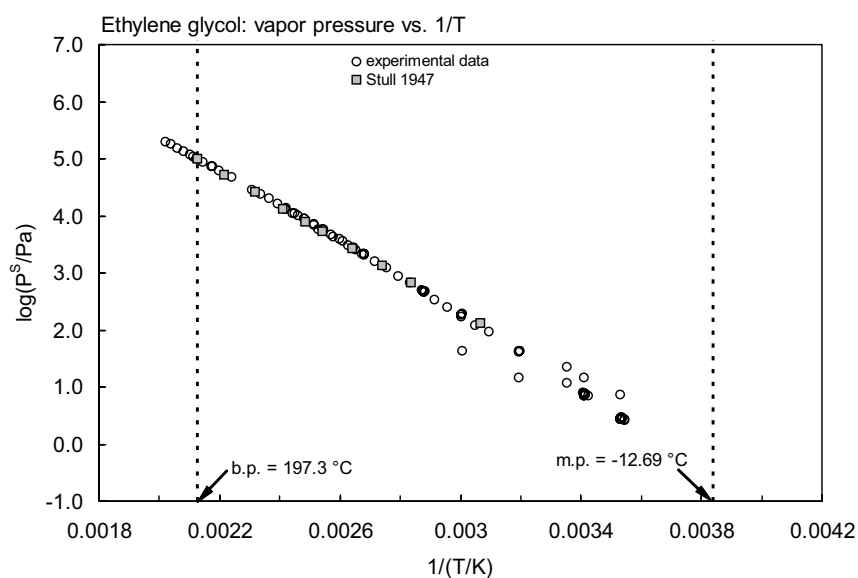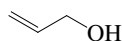| Stull 1947 | | Ambrose & Hall 1981 | | Hales et al. 1981 | | | |
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		(extrapolated value)				A	23.7259
						B	4648.55
		bp/°C	297.54			C	503391
		eq. 3	P/kPa				
		A	6.83995				
		B	1818.591				
		C	–94.499				

FIGURE 11.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for ethylene glycol.

11.1.1.16 Allyl alcohol

Common Name: Allyl alcohol
Synonym: propenylalcohol, 2-propen-1-ol, 1-propene-3-ol, vinylcarbinol
Chemical Name: allyl alcohol, 1-propene-3-ol, 2-propen-1-ol
CAS Registry No: 107-18-6
Molecular Formula: C_3H_6O, $CH_2=CHCH_2OH$
Molecular Weight: 58.079
Melting Point (°C):
 –129 (Stull 1947; Weast 1982–83; Verschueren 1983; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
 97.1 (Weast 1982–83; Dean 1985; Riddick et al. 1986)
 97 (Lide 2003)
Density (g/cm³ at 20°C):
 0.854 (Weast 1982–83; Dean 1985)
 0.85511 (15°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
 64.8 (Kamlet et al. 1986; Leahy 1986)
 74.0 (calculated-Le Bas method at normal boiling point)
Acid Dissociation Constant, pK_a:
 15.5 (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
 miscible (Dean 1985)
 miscible (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 2666* (21.7°C, temp range –20 to 96.6°C, Stull 1947)
 3140 (Hoy 1970)
 log (P/mmHg) = [–0.2185 × 10577.7/(T/K)] + 9.143231; temp range –20 to 96.6°C (Antoine eq., Weast 1972–73)
 2666, 4266 (20°C, 30°C, Verschueren 1983)
 3750 (Riddick et al. 1986)
 log (P/kPa) = 31.75070 – 3451.8/(T/K) – 7.94975 log (T/K); temp not specified (Riddick et al. 1986)
 3298 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 log (P_L/kPa) = 7.40725 – 1790.13/(–38.295 + T/K); temp range 253–370 K (Antoine eq., Stephenson & Malanowski 1987)
 log (P/mmHg) = 21.3978 – 2.9525 × 10³/(T/K) – 3.8137·log(T/K) – 2.7145 × 10⁻³·(T/K) + 1.8811 × 10⁻⁶·(T/K)²; temp range 144–545 K (vapor pressure eq., Yaws 1994)
 6954* (38.28°C, ebulliometry, measured range 311.42–355.70 K, Lubomska & Malanowski 2004)
 log (P/kPa) = 6.936209 – 1513.129/[(T/K) – 63.131]; temp range 311.42–355.70 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry's Law Constant (Pa·m³/mol at 25°C):
 0.506 (calculated-C_W/C_A., Hine & Mookerjee 1975)
 0.510 (calculated-bond contribution, Hine & Mookerjee 1975)
 0.564 (computed, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
- 0.17   (shake flask, Hansch & Leo 1979)
- 0.17   (recommended, Sangster 1989)
- 0.17   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

    Hydrolysis:

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

        photooxidation $t_{1/2}$ = 334 d-37 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991)

        photooxidation $t_{1/2}$ = 2.2–22 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

        k_{OH} = 25.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 440 K (Atkinson 1989)

    Biodegradation: $t_{1/2}$(aq. aerobic) = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Sasaki 1978; quoted, Howard et al. 1991); $t_{1/2}$(aq. anaerobic) = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

    Biotransformation:

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

Half-Lives in the Environment:

    Air: photooxidation $t_{1/2}$ = 2.2–22 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

    Surface water: photooxidation $t_{1/2}$ = 334 d-37 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991).

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

    Sediment:

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

    Biota:

TABLE 11.1.1.16.1
Reported vapor pressures of allyl alcohol at various temperatures

Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
t/°C	P/Pa	T/K	P/Pa
–20.0	133.3	311.42	6954
0.20	666.6	315.81	8869
10.5	1333	319.97	11079
21.7	2666	326.70	15672
33.4	5333	331.84	20194
40.3	7999	334.20	22603
50.0	13332	337.96	26943
64.5	26664	341.54	31723

TABLE 11.1.1.16.1 *(Continued)*

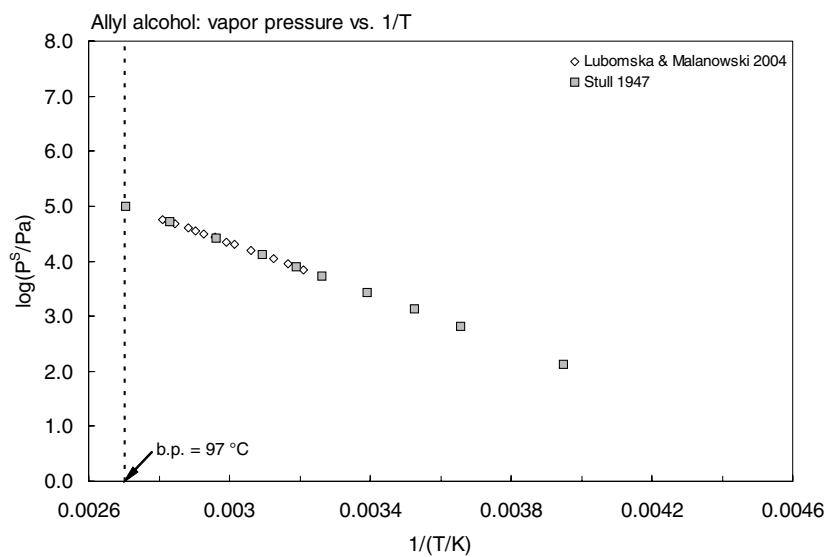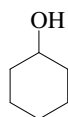| Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
t/°C	P/Pa	T/K	P/Pa
80.2	53329	344.27	35822
96.6	101325	346.97	40304
		351.37	48613
mp/°C	−129	353.15	52334
		353.59	53299
		355.70	58108

FIGURE 11.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for allyl alcohol.

11.1.1.17   Cyclohexanol

Common Name: Cyclohexanol
Synonym: adronol, anol, cyclohexylalcohol, hexahydrophenol, hexalin, hydralin, hydrophenol
Chemical Name: cyclohexanol
CAS Registry No: 108-93-0
Molecular Formula: $C_6H_{11}OH$
Molecular Weight: 100.158
Melting Point (°C):
    25.93   (Lide 2003)
Boiling Point (°C):
    160.84   (Lide 2003)
Density (g/cm^3):
    0.9624   (Lide 2003)
Molar Volume (cm^3/mol):
    104.0   (calculated-density, Lande & Banerjee 1981)
    125.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    1.70   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section):
    37000*   (shake flask-synthetic method, temp range 7.2–184.72°C, Sidgwick & Sutton 1930)
    39200   (shake flask-interferometry, Hansen et al. 1949)
    32920   (residue volume, Booth & Everson 1942)
    40000*   (20°C, synthetic method, measured range 0–184°C, Zil'berman 1951)
    48960   (shake flask-interferometry, Donahue & Bartell 1952)
    36000   (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
    38000*   (recommended "best" value, IUPAC Solubility Data Series, temp range 0–180°C, Baron 1984)
    37500   (selected, Riddick et al. 1986)
    44400*   (19.7°C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson & Stuart 1986)
    38200   (selected, Yaws et al. 1990)
    37500   (dialysis tubing equilibration-GC. Etzweiler et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    467*   (34.0°C, Ramsay-Young method, measured range 34.0–149.0°C, Gardner & Brewer 1937)
    133.1*, 194 (21°C, interpolated-regression of tabulated data, temp range 21–161°C, Stull 1947)
    7177*   (93.73°C, temp range 93.73–160.70°C, Novak et al. 1960; quoted, Boublik et al. 1984)
    log (P/mmHg) = [–0.2185 × 11935.8/(T/K)] + 8.909086; temp range 21–161°C (Antoine eq., Weast 1972–73)
    174.8   (calculated-Cox eq., Chao et al. 1983)
    log (P/mmHg) = [1– 434.658/(T/K)] × 10^{0.951396 – 8.46102 × 10^{-4}·(T/K) + 8.87926 × 10^{-7}·(T/K)^2}; temp
        range 294.15–434.15 K (Cox eq., Chao et al. 1983)
    37.53   (extrapolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 6.2553 – 912.87/(109.13 + t/°C); temp range 94–161°C (Antoine eq., Dean 1985, 1992)
    1300   (56°C, Riddick et al. 1986)
    log (P/kPa) = 5.92859 – 1199.10/(t/°C + 145.0); temp range 107–160°C (Riddick et al. 1986)
    97.36   (interpolated, solid, Antoine eq.-I, Stephenson & Malanowski 1987)

80.0, 84.85 (extrapolated, liquid, Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 9.631 - 3173.1/(T/K)$; temp range 272–298 K (Antoine eq.-I, for solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.1634 - 1318.5/(-116.55 + T/K)$; temp range 318–434 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.27792 - 1381.8/(-110.132 + T/K)$; temp range 300–434 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

106.6   (Daubert & Danner 1989)

14.66, 196.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/mmHg) = 49.9123 - 4.8446 \times 10^3/(T/K) - 13.711 \cdot \log(T/K) + 3.5451 \times 10^{-9} \cdot (T/K) + 1.5932 \times 10^{-6} \cdot (T/K)^2$; temp range 297–625 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):

0.581   (calculated-C_W/C_A., Hine & Mookerjee 1975)

2.48, 2.37   (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

0.281   (calculated-P/C, Howard 1993)

0.278   (correlated-molecular structure, Russell et al. 1992)

0.446   (wetted-wall column-GC, Altschuh et al. 1999)

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

1.23   (shake flask-AS, Hansch & Anderson 1967, Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)

1.36   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

1.23   (recommended, Sangster 1989, 1993)

1.23   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.708   (estimated-K_{OW}, Lyman et al. 1990)

0.176   (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

2.045   (soil, estimated-K_{OW}, Lyman et al. 1990; quoted, Howard 1993)

1.114   (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

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

Volatilization: $t_{1/2}$ ~145 d estimated from a model environmental pond with the consideration of the effect of adsorption (USEPA 1987; quoted, Howard 1993);

based on the Henry's law constant, $t_{1/2}$ ~13.3 d from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s at 25°C (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

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

$k_{OH} = 17.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with OH radical concentration of 5×10^5 per cm^3 in air at 25°C corresponds to an atmosphere $t_{1/2}$ = 22 h (Atkinson 1987; quoted, Howard 1993)

Hydrolysis:

Biodegradation: average rate of biodegradation k = 28.0 mg COD g^{-1} h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

   Air: photooxidation $t_{1/2}$ = 22 h, based on estimated reaction rate constant of 17.4×10^{-12} cm^3 molecule^{-1} s^{-1} for
        the vapor phase reaction with 5×10^5 hydroxyl radical per cm^3 in air at 25°C (Howard 1993).
   Surface water:
   Ground water:
   Sediment:
   Soil:
   Biota:

TABLE 11.1.1.17.1
Reported aqueous solubilities of cyclohexanol at various temperatures

| Sidgwick & Sutton 1930		Zil'berman 1951		Barton 1984		Stephenson & Stuart 1986	
synthetic method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
7.2	50000	0	53400	0	53000	0	67700
9.4	47800	10	45700	10	46200	9.5	54000
9.7	45800	20	40000	20	39700	19.7	44400
11.2	44100	30	36000	25	38000	30.6	37400
12.0	45500	40	33300	30	35500	40.0	36300
14.2	42300	50	31400	40	33000	50.0	34900
15.2	42900	54	31000	50	31000	60.3	33700
16.3	40900	62	31000	60	31000	70.1	34400
20.6	39500	70	31900	70	32000	80.2	36000
20.8	38200	80	34100	80	34000	90.3	37500
24.6	.37500	90	36500	90	37000		
27.55	35200	100	39300	100	39000		
28.7	35700	110	42800	110	43000		
31.85	33700	120	47000	120	49000		
33.6	34100	130	53000	130	56000		
40.4	32600	140	61000	140	64000		
40.45	31800	150	72000	150	77000		
45.8	31900	160	88000	160	93000		
121.95	51400	170	115000	170	120000		
156.9	92200	180	178000	180	190000		
174.3	150000	184	339000				
179.4	192000						
184.72	324000						
		Zh. Fis. Khim. 24, 776–8					
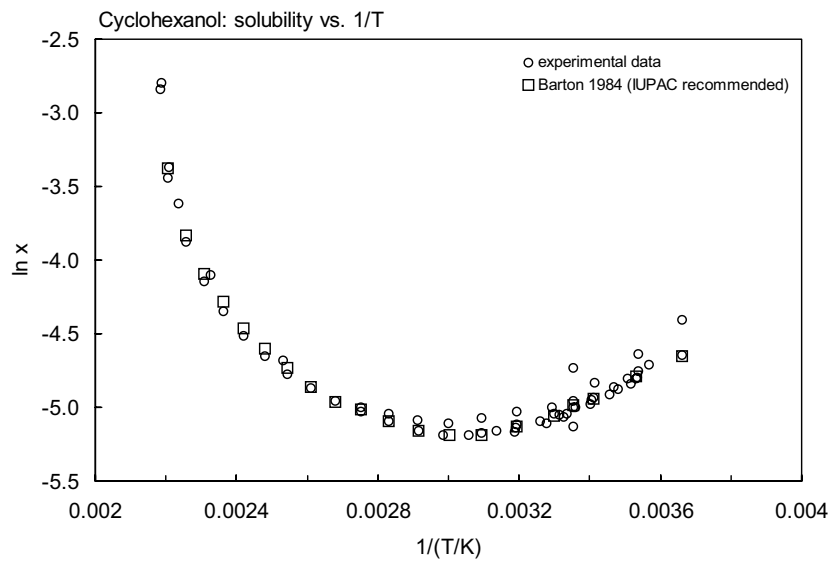
FIGURE 11.1.1.17.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclohexanol.

TABLE 11.1.1.17.2
Reported vapor pressures of cyclohexanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(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)		

| Gardner & Brewer 1937		Stull 1947		Novak et al. 1960	
Ramsay-Young method		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
34.0	467	21.0	133.3	93.73	7177
37.5	560	44.0	666.6	97.02	9210
46.4	587	56.0	1333	99.71	10426
47.8	693	68.8	2666	102.52	11876
53.6	907	83.0	5333	104.83	13159
59.4	1133	91.8	7999	108.82	15372
73.0	2773	103.7	13332	112.70	18252
80.5	4146	121.7	26664	116.86	21891
97.8	9826	141.4	53329	120.35	25264
119.1	13771	161.0	101325	125.54	30864
136.9	47036			130.95	37543
149.0	71994	mp/°C	23	136.22	45356
				142.41	56448
bp/°C	162.3			148.72	69487
				155.71	86046
				160.70	99192
				in Boublik et al. 1984	
				eq. 2	P/kPa
				A	5.34182
				B	894.818
				C	106.797
				bp/°C	161.425
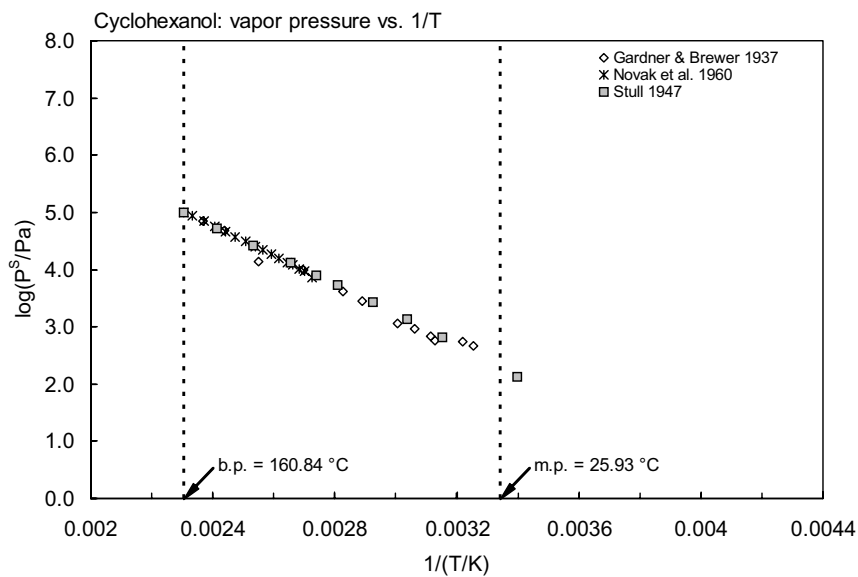
FIGURE 11.1.1.17.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanol.

11.1.1.18 Benzyl alcohol
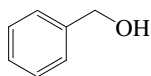
Common Name: Benzyl alcohol
Synonym: benzenemethanol, (hydroxymethyl)benzene, *o*-hydroxy toluene, phenylcarbinol, phenylmethanol
Chemical Name: benzyl alcohol
CAS Registry No: 100-51-6
Molecular Formula: C_7H_8O, $C_6H_5CH_2OH$
Molecular Weight: 108.138
Melting Point (°C):
    –15.4   (Lide 2003)
Boiling Point (°C):
    205.31   (Lide 2003)
Density (g/cm^3 at 20°C):
    1.04535, 1.04156   (20°C, 25°C, Dreisbach 1955)
    1.04127   (25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
    103.5   (calculated-density, Rohrschneider 1973)
    125.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    48.13, 61.42   (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    17.406   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/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):
    38020   (Seidell 1941)
    34200   (estimated, McGowan 1954)
    38000   (20–25°C, shake flask-GC, Urano et al. 1982)
    35000   (20°C, Verschueren 1983)
    42900   (shake flask-LSC, Banerjee 1985)
    43000*   (20.1°C, shake flask-GC/TC, measured range 0–50°C, Stephenson & Stuart 1986)
    46070   (shake flask-GC, Li et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    133.3*   (60.9°C, static method, measured range 60.9–152.1°C, Kahlbaum 1898)
    26.7*   (38.8°C, ebulliometry, measured range 38.8–151.6°C, Gardner & Brewer 1937)
    15.40*   (extrapolated-regression of tabulated data, temp range 58–205.7°C, Stull 1947)
    log (P/mmHg) = 7.90550 – 2187.8/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    6287*   (122.52°C, ebulliometry, measured range 122.52–205.41°C, Dreisbach & Shrader 1949)
    19.59   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 7.58200 – 1904.3/(200.0 + t/°C); temp range 112–330°C (Antoine eq. for liquid state, Dreisbach 1955)
    12.0   (Hoy 1970)
    log (P/mmHg) = [–0.2185 × 14093.2/(T/K)] + 9.391874; temp range 58–204.7°C (Antoine eq., Weast 1972–73)
    8.35*, 10.06 (20°C, 25°C, extrapolated-Antoine eq., gas-saturation method, Grayson & Fosbraey 1982)
    log (P/Pa) = 29.0 – 7958/(T/K); temp range 29.5–60.1°C (Antoine eq., gas saturation, Grayson & Fosbraey 1982)
    4.750   (extrapolated-Cox eq., Chao et al. 1983)

log (P/mmHg) = [1– 479.624/(T/K)] × 10^{1.02742 – 6.26739 × 10^{-4}·(T/K) + 1.28791 × 10^{-7}·(T/K)^2}; temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)

12.07, 9.69 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.34897 – 1650.313/(174.623 + t/°C); temp range 122.5–205.4°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P/kPa) = 6.39383 – 1655.003/(171.85 + t/°C); temp range 38.8–151.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11.72 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.19817 – 1632.593/(172.79 + t/°C); temp range 122–205°C (Antoine eq., Dean 1985, 1992)

15.0 (selected, Riddick et al. 1986)

log (P/kPa) = 8.963 – 3214/(T/K); temp range not specified (Antoine eq., Riddick et al. 1986)

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

log (P$_L$/kPa) = 6.7069 – 1904.3/(–73.15 + T/K); temp range 385–573 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 8.963 – 3214/(T/K); temp range 293–315 K (Antoine eq-II., Stephenson & Malanowski 1987)

7.395 (ebulliometry, fitted to Antoine eq., Ambrose & Ghiassee 1990)

12.0 (calculated-Wagner eq., Ambrose & Ghiassee 1990)

log (P/mmHg) = –36.2189 – 3.3475 × 10^3/(T/K) + 23.337·log(T/K) – 4.46 × 10^{-2}·(T/K) + 2.1443 × 10^{-5}·(T/K)^2; temp range 258–677 K (vapor pressure eq., Yaws 1994)

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

0.0231 (quoted estimated value of Hine & Mookerjee 1975, Howard 1993)

0.0396 (calculated-P/C, Howard 1993)

< 0.0273 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K$_{OW}$:

1.10 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968)

1.10 ± 0.02 (shake flask-UV, Iwasa et al. 1965)

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

1.10 (shake flask-RC, Cornford 1982)

1.00 (shake flask-UV, Mayer et al. 1982)

1.16 ± 0.02 (exptl.-ALPM, Garst & Wilson 1984)

1.06 (HPLC-k' correlation, Eadsforth 1986)

1.58 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

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

1.05 (recommended, Sangster 1989, 1993)

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

0.96 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)

1.10 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

0.602 (calculated-K$_{OW}$, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K$_{OC}$:

1.193 (red-brown Australian soil with 1.09% organic carbon, Briggs 1981; quoted, Howard 1993)

0.790 (calculated-K$_{OW}$, Kollig 1993)

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

Volatilization: estimated t$_{1/2}$ = 97 d for a model river of 1 m deep, flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

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

$k_{OH} = 22.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1989)

k_{OH}(calc) = 7.99×10^{-12} cm^3 molecule^{-1} s^{-1}, estimated from Atmospheric Oxidation Program; k_{OH}(exptl) = 22.9×10^{-12} cm^3 molecule^{-1} s^{-1}; and k_{OH}(calc) = 7.98×10^{-12} cm^3 molecule^{-1} s^{-1}, estimated from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

k_{OH}(calc) - 0.85×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(exptl) = 22.9×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant k = 0.042–0.062 h^{-1} in 30 mg L^{-1} activated sludge after a lag time of 5–15 h (Urano & Kato 1986).

Biotransformation:

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

Half-Lives in the Environment:

Air: the estimated $t_{1/2}$ ~2 d for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.18.1
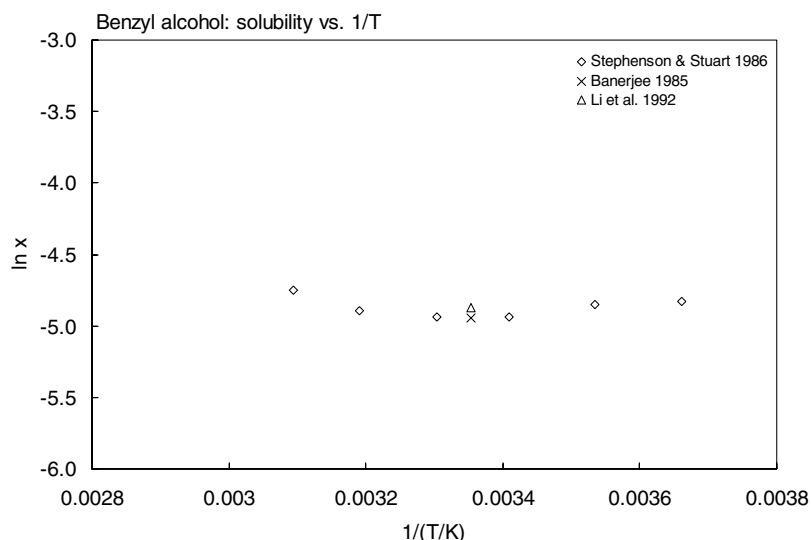**Reported aqueous solubilities of benzyl alcohol at various temperatures**

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	S/g·m^{-3}
0	48000
9.8	47000
20.1	43000
29.6	43000
40.2	45000
50.0	52000

FIGURE 11.1.1.18.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzyl alcohol.

TABLE 11.1.1.18.2
Reported vapor pressures of benzyl alcohol 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)		

Kahlbaum 1898		Gardner & Brewer 1937		Stull 1947		Grayson & Fosbraey 1982	
static method		ebulliometry		summary of literature data		gas saturation-GC/LC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
60.9	133.3	38.8	26.7	58.0	133.3	29.5	18.29
67.8	266.6	42.5	80.0	80.8	666.6	30.2	22.77
72.9	400.0	46.8	106.7	92.6	1333	39.8	44.22
77.2	533.3	50.5	120.0	105.8	2666	40.1	46.11
80.8	666.6	85.2	906.6	119.8	5333	49.7	101.41
92.8	1333.2	97.2	1747	129.3	7999	60.1	221.10
99.9	1999.8	113.5	3880	141.7	13332	20	8.35
105.3	2666.4	128.8	7786	160.0	26664		
109.7	3333.06	151.6	18918	183.0	53329	eq. 1a	P/Pa
113.4	3999.7			204.7	101325	A	29.0
116.7	4666.3	bp/°C	206.9			B	7958
119.6	5332.9			mp/°C	–15.3		
122.2	5999.5						
124.4	6666.1						
133.9	9999.2			**Dreisbach & Shrader 1949**			
141.3	13332			ebulliometry			
152.1	19998			t/°C	P/Pa		
				122.52	6287		
				127.12	7605		
				130.90	8851		
				134.28	10114		
				147.09	16500		
				190.50	67661		
				205.41	101325		
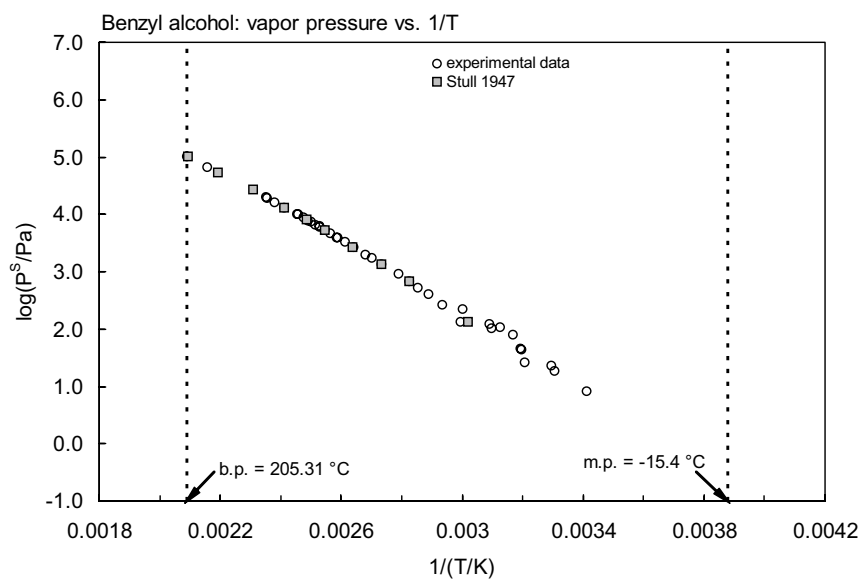
FIGURE 11.1.1.18.2 Logarithm of vapor pressure versus reciprocal temperature for benzyl alcohol.

TABLE 11.2.1
Summary of physical properties of alcohols

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 MW/ρ at 20°C	Le Bas
Methanol	67-56-1	CH_3OH	32.042	−97.53	64.6	1	40.49	37.0
Ethanol	64-17-5	C_2H_5OH	46.068	−114.14	78.29	1	58.36	59.2
Propanol (*n*-Propyl alcohol)	71-23-8	C_3H_7OH	60.095	−124.39	97.2	1	74.79	81.4
Isopropanol (*i*-Propyl alcohol)	67-63-0	iC_3H_7OH	60.095	−87.9	82.3	1	76.51	81.4
1-Butanol (*n*-Butyl alcohol)	71-36-3	C_4H_9OH	74.121	−88.6	117.73	1	91.56	103.6
Isobutanol (*i*-Butyl alcohol)	78-83-1	iC_4H_9OH	74.121	−101.9	107.89	1	92.47	103.6
sec-Butyl alcohol	78-92-2	sC_4H_9OH	74.121	−88.5	99.51	1	91.90	103.6
tert-Butyl alcohol	75-65-0	tC_4H_9OH	74.121	25.69	82.4	1	94.88	103.6
1-Pentanol (*n*-Amyl alcohol)	71-41-0	$C_5H_{11}OH$	88.148	−77.6	137.98	1	108.23	125.8
2-Pentanol	6032-29-7	$C_5H_{11}OH$	88.148	−73	119.3	1	108.91	125.8
1-Hexanol	111-27-3	$C_6H_{13}OH$	102.174	−47.4	157.6	1	124.79	148.0
1-Heptanol	111-70-6	$C_7H_{15}OH$	116.201	−33.2	176.45	1	141.38	170.2
1-Octanol (*n*-Octyl alcohol)	111-87-5	$C_8H_{17}OH$	130.228	−14.8	195.16	1	157.85	192.4
1-Nonanol	143-08-8	$C_9H_{19}OH$	144.254	−5	213.37	1	174.37	214.6
1-Decanol	112-30-1	$C_{10}H_{21}OH$	158.281	6.9	231.1	1	190.77	236.8
Ethylene glycol	107-21-1	$(CH_2OH)_2$	62.068	−12.69	197.3	1	55.98	66.6
Allyl alcohol	107-18-6	C_3H_5OH	58.079	−129	97	1	67.92	74.0
Cyclopentanol	96-41-3	C_5H_9OH	86.132	−17.5	140.42	1	90.78	106.9
Cyclohexanol	108-93-0	$C_6H_{11}OH$	100.158	25.93	160.84	1	104.07	125.6
Benzyl alcohol	100-51-6	C_7H_7OH	108.138	−15.4	205.31	1	103.85	125.6

TABLE 11.2.2
Summary of selected physical-chemical properties of alcohols at 25°C

| Compound | Selected properties | | | log K_{OW} | Henry's law constant H/(Pa·m³/mol) | | | |
| | Solubility | | Vapor pressure | | | | | |
	S/(g/m³)	C_L/(mol/m³)	P_L/Pa		calcd P/C	exptl (a)	exptl (b)	exptl (c)
Methanol	miscible	miscible	16210	–0.77		0.45		0.45
Ethanol	miscible	miscible	7800	–0.31		0.53		0.527
Propanol	miscible	miscible	2780	0.25				0.751
Isopropanol	miscible	miscible	5700	0.05				0.80
1-Butanol	74000	998.4	900	0.82	0.9014	0.80	0.892	0.80
Isobutanol	81000	1093	1500	0.76	1.3726	0.99		0.99
sec-Butyl alcohol	181000	2442	2300	0.61	0.9419	0.80		0.918
tert-Butyl alcohol	miscible	miscible	5500	0.35		1.46		1.46
1-Pentanol	22000	249.6	300	1.50	1.202	1.314		
2-Pentanol	45000	510.5	777	1.14	1.522			
1-Hexanol	6000	58.72	110	2.03	1.873	1.562	1.735	
1-Heptanol	1740	14.97	24	2.62	1.603	1.909		
1-Octanol	540	4.146	11	3.07	2.653	2.454	2.48	
1-Nonanol	130	0.9012		4.26				
1-Decanol	37	0.2338		4.57				
Ethylene glycol	miscible	miscible	12	–1.36		0.006		
Allyl alcohol	miscible	miscible	3750	0.17				
Cyclopentanol			292					
Cyclohexanol	38000	379.4	85	1.23	0.224			
Benzyl alcohol	80	0.7398	12	1.10	16.22			

(a) Butler et al. 1935

(b) Buttery et al. 1969

(c) Snider & Dawson 1985

TABLE 11.2.3
Suggested half-life classes of alcohols in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Methanol	4	3	3	4
Ethanol	3	3	3	4
Propanol (*n*-Propyl alcohol)	3	3	3	4
Isopropanol (*i*-Propyl alcohol)	3	3	3	4
1-Butanol (*n*-Butyl alcohol)	3	3	3	4
Isobutanol (*i*-Butyl alcohol)	3	3	3	4
tert-Butyl alcohol	4	4	4	5
1-Pentanol (*n*-Amyl alcohol)	3	3	3	4
1-Hexanol	3	3	3	4
1-Octanol (*n*-Octyl alcohol)	3	3	3	4
Ethylene glycol	3	3	3	4
Allyl alcohol	3	3	3	4
Cyclohexanol	3	3	3	4
Benzyl alcohol	3	3	3	4

where,

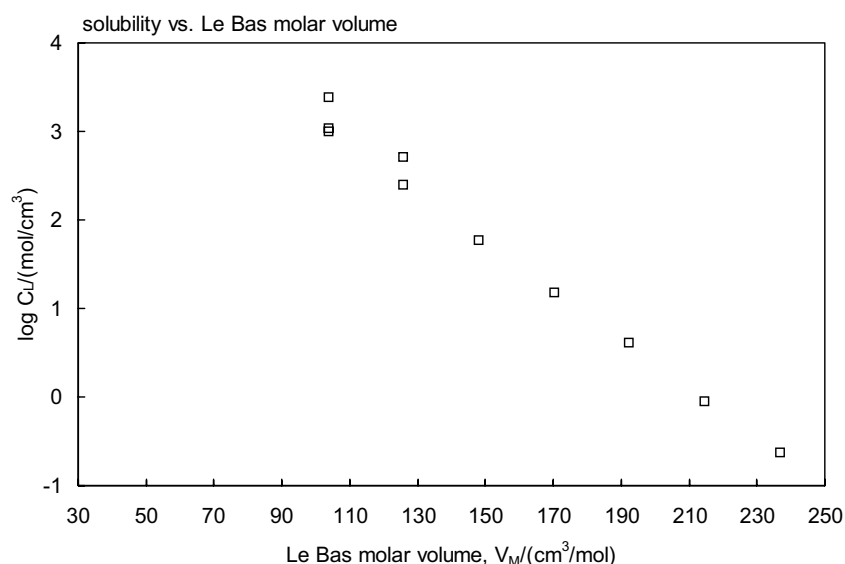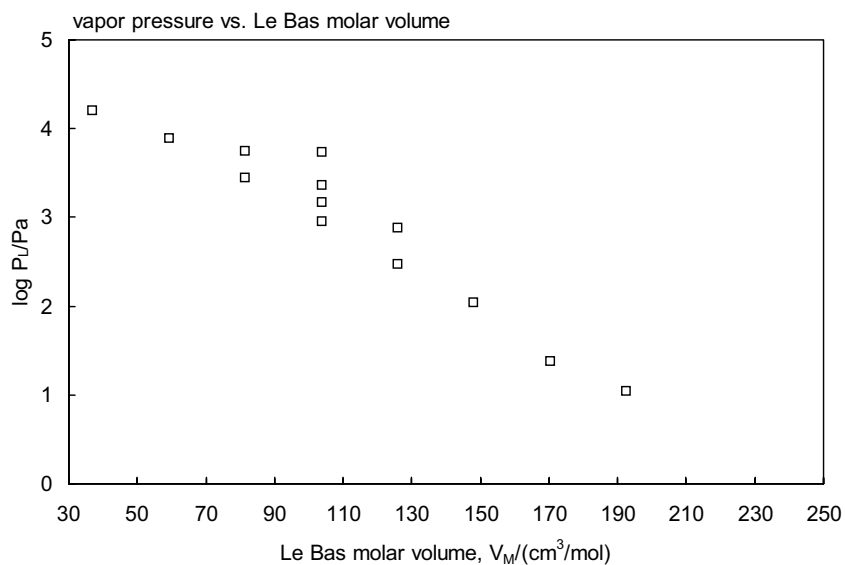| Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

FIGURE 11.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.
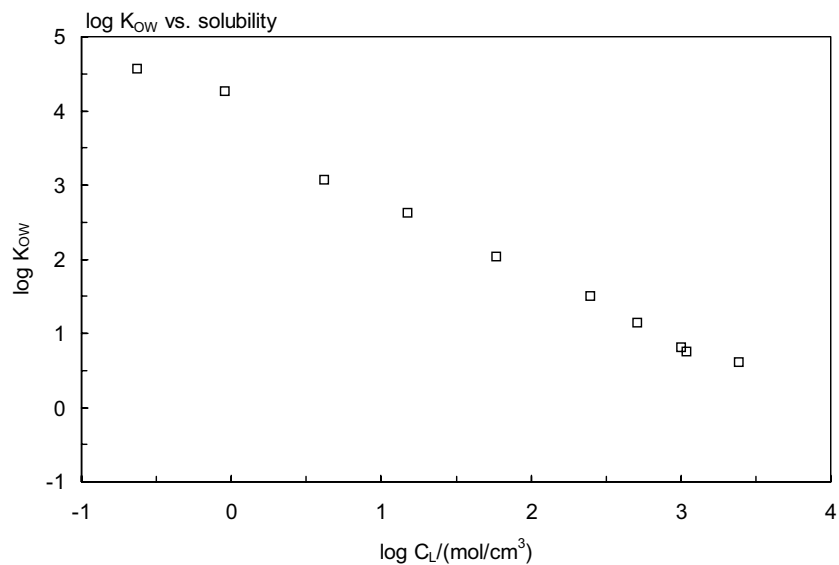
FIGURE 11.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.
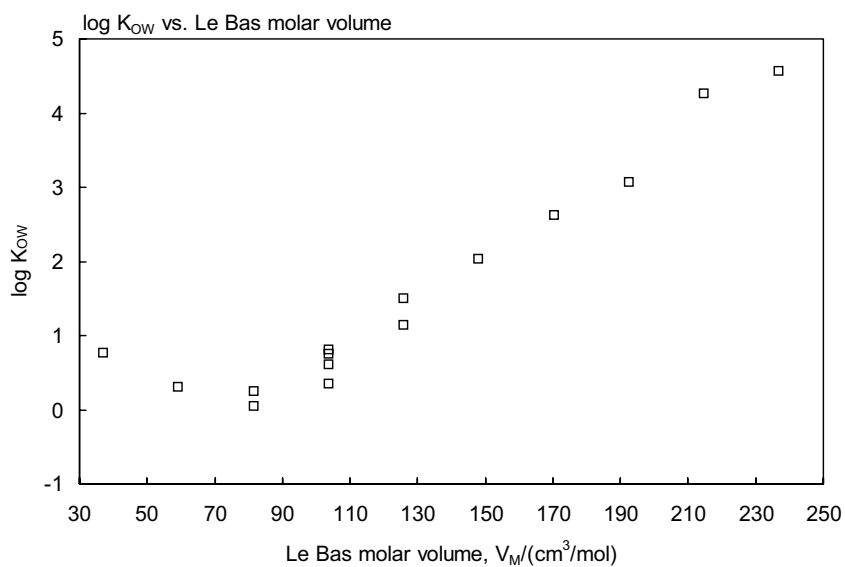
FIGURE 11.2.3 Octanol-water partition coefficient versus Le Bas molar volume for alcohols.

Henry's law constant vs. Le Bas molar volume
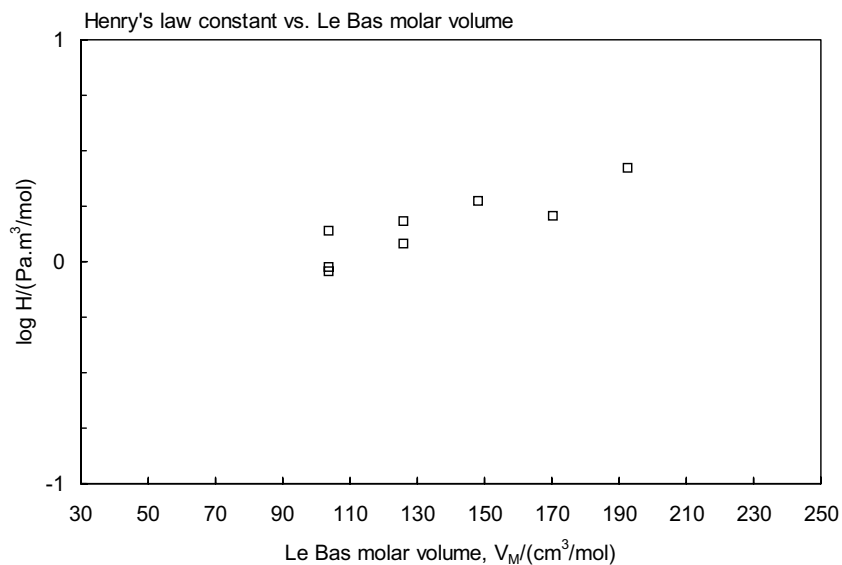
FIGURE 11.2.4 Henry's law constant versus Le Bas molar volume for alcohols.

log K$_{OW}$ vs. solubility

FIGURE 11.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alcohols.

11.3 REFERENCES

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