
13 Carboxylic Acids

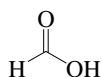
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13.1 LIST OF CHEMICALS AND DATA COMPILATIONS

13.1.1 ALIPHATIC ACIDS

13.1.1.1 Formic acid



Common Name: Formic acid

Synonym: methanoic acid

Chemical Name: formic acid

CAS Registry No: 64-18-6

Molecular Formula: CH_2O_2 , HCOOH

Molecular Weight: 46.026

Melting Point ($^{\circ}\text{C}$):

8.3 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

101 (Lide 2003)

Density (g/cm^3 at 20°C):1.21961, 1.21328 (20°C , 25°C , Dreisbach & Martin 1949)

1.2200 (Weast 1982–83; Dean 1985)

1.2141 (25°C , Riddick et al. 1986)Molar Volume (cm^3/mol):

37.7 (calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :3.751 (pK_a , Dean 1985)3.752 (pK_a , Riddick et al. 1986)3.740 (pK_a , Sangster 1989)

3.800 (Kollig 1993)

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

12.68 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 13.5 \text{ J}/\text{mol K}$), F: 1.0Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

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

4344* (24.6°C , temp range 21.8 – 100.6°C , Kahlbaum 1894)5333* (24°C , compiled and evaluated data, temp range -20 to 100.6°C , Stull 1947) $\log (P/\text{mmHg}) = 7.15689 - 1414.1/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)10114* (37.75°C , ebulliometry, measured range 37.75 – 100.7°C , Dreisbach & Shrader 1949) $\log (P/\text{mmHg}) = [-0.2185 \times 9896.5/(T/\text{K})] + 8.779337$; temp range -20 to 100.6°C (Antoine eq., Weast 1972–73)4666, 7198 (20°C , 30°C , Verschuereen 1983)

5720, 5744, 4420 (calculated-Antoine eq., Boublik et al. 1984)

 $\log (P/\text{kPa}) = 4.09278 - 539.775/(136.826 + t/^{\circ}\text{C})$; temp range 0.5 – 34.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984) $\log (P/\text{kPa}) = 6.69157 - 1689.096/(259.726 + t/^{\circ}\text{C})$; temp range 37.35 – 100.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984) $\log (P/\text{kPa}) = 3.7279 - 295.021/(70.7 + t/^{\circ}\text{C})$; temp range 21 – 100.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 5744 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.5818 - 1699.2/(260.7 + t/^{\circ}\text{C})$; temp range: 37–101°C (Antoine eq., Dean 1985, 1992)
 5750 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.50280 - 1563.28/(247.06 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 5733* (comparative ebulliometry, measured range 299.8–393 K, Ambrose & Ghiassee 1987)
 $\ln (P/\text{kPa}) = 15.40560 - 3894.764/[(T/\text{K}) - 13.0]$; temp range 299.8–393 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghiassee 1987)
 5711 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.611 - 3160/(T/\text{K})$; temp range 268–281 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5028 - 1563.28/(-26.09 + T/\text{K})$; temp range 283–384 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 5680, 67850 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 27.9278 - 2.5976 \times 10^3/(T/\text{K}) - 7.2489 \cdot \log (T/\text{K}) + 6.411 \times 10^{-10} \cdot (T/\text{K}) + 3.9421 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 282–580 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

- 0.0181 (calculated, Keene & Galloway 1986)
 0.0274 (calculated, Jacob 1986)
 0.017 (pH 4, Gaffney et al. 1987)
 0.112 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0076, 0.0098, 0.0178 (24°C, bubble column technique, concn: of 1, 10, 10⁵ ppm, Servant et al. 1991)
 0.0281 (Betterton 1992)
 0.018 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [k_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -10.31 + 5634/(T/\text{K})$, temp range 178.15–308.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0183 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.018–0.028 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0118, 0.00921 (counter-flow packed column technique-ion chromatography; "best" exptl. value, Johnson et al. 1996)
 $\ln [k_H/(\text{M/atm})] = -11.04 + 6100/(T/\text{K})$; temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)
 0.0137 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 0.0107 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.914 - 2425/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- −0.54 (shake flask-titration, Collander 1951; quoted, Leo et al. 1971; Hansch et al. 1972; Hansch & Leo 1979)
 −0.54 (shake flask-titration, Whitehead & Geankoplis 1955)
 −0.46 (calculated-f const., Rekker & de Kort 1979)
 −0.54 (recommended, Sangster 1989)
 −0.54 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

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

- −0.27 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Hydrolysis:

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

$k_{\text{OH}} = (3.2 \pm 1.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982)

$k = (100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ at pH 8; $(5 \pm 5) \text{ M}^{-1} \text{ s}^{-1}$ for protonated species; $(100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0–4.0 and 20–23°C (Hoigné & Bader 1983b)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–430 K (flash photolysis-resonance fluorescence, Wine et al. 1985)

$k_{\text{OH}} = (2.95 \pm 0.07) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance absorption, Jolly et al. 1986)

$k_{\text{OH}} = (3.7 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{\text{OH}}^* = (2.69 \pm 0.17) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–445 K (laser photolysis-resonance absorption, Singleton et al. 1988)

$k_{\text{OH}} = 3.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k(\text{soln}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 13.1.1.1.1

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

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

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3) \quad \ln (P/\text{Pa}) = A - B/(C + T/K) \quad (3a)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Kahlbaum 1894		Stull 1947		Dreisbach & Shrader 1949		Ambrose & Ghiassie 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
21.8	3312	−20.0	133	37.75	10114	299.789	6188
22.6	3688	−5.0	666.6	48.79	16500	302.006	6876
24.6	4344	2.10	1333	73.55	42066	307.578	8881
27.9	5520	10.3	2666	87.82	67661	308.389	9230
30.5	6621	24.0	5333	100.7	101325	310.035	9896
37.8	9938	32.4	7999			313.764	11668
100.6	101325	43.8	13332	bp/°C	100.7	316.803	13293
		61.4	26664			319.729	15031
		80.3	53329			324.842	18432
		100.6	101325			326.895	20105
						329.030	21830
		mp/°C	8.2			332.807	25236
						336.159	28640
						342.086	35456
						344.582	38845
						346.997	43226
						349.134	45630

TABLE 13.1.1.1.1 (Continued)

Kahlbaum 1894		Stull 1947		Dreisbach & shrader 1949		Ambrose & Ghiassee 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
						350.313	47321
						353.362	52449
						355.215	55868
						↓	↓
						392.654	172035
						298.15	5733
						Antoine eq.	
						eq. 3a	P/kPa
						A	15.40560
						B	3894.764
						C	−13.0
						bp/K	374.04

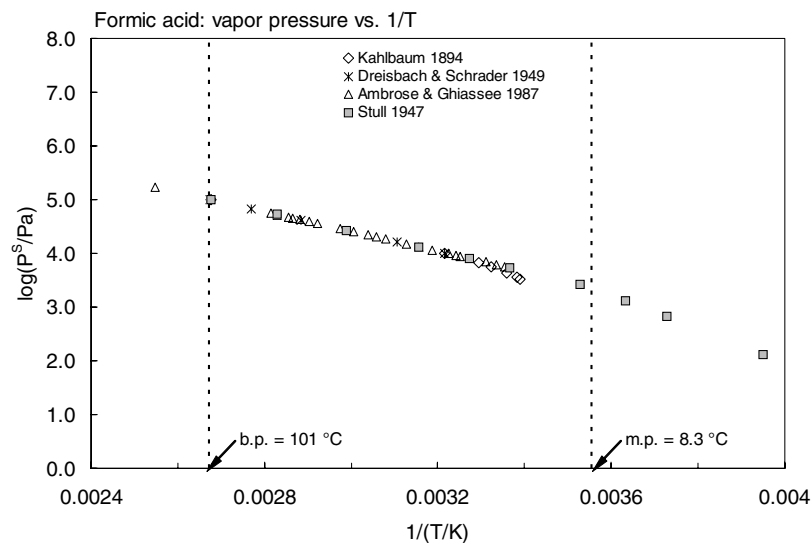


FIGURE 13.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for formic acid.

13.1.1.2 Acetic acid



Common Name: Acetic acid

Synonym: ethanoic acid, methanecarboxylic acid, glacial acetic, vinegar acid

Chemical Name: acetic acid

CAS Registry No: 64-19-7

Molecular Formula: CH_3COOH

Molecular Weight: 60.052

Melting Point ($^{\circ}\text{C}$):

16.64 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

117.9 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at 20°C):

1.04923, 1.04365 (20°C , 25°C , Dreisbach & Martin 1949)

1.0492 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

57.1 (calculated-density, Rohrschneider 1973)

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

Dissociation Constant, pK_a :

4.733 (pK_a , Korman & La Mer 1936)

4.760 (pK_a , Fieser & Fieser 1958; Sangster 1989)

4.750 (pK_a , Weast 1982–83; Howard 1990)

4.756 (pK_a , Dean 1985; Riddick et al. 1986)

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

11.72 (Ambrose et al. 1977; Riddick et al. 1986)

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

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

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

miscible (Dean 1985; Riddick et al. 1986)

miscible (Yaws et al. 1990)

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

2040* (interpolated-regression of tabulated data, temp range -17.2 – 118°C , Stull 1947)

$\log(P/\text{mmHg}) = 7.45144 - 1589.3/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

10114* (55.75°C , ebulliometry, measured range 55.75 – 117.72°C , Dreisbach & Shrader 1949)

2666* (29.8°C , static method-manometer, measured range 29.8 – 126.45°C , Potter & Ritter 1954)

8297* (52.36°C , ebulliometry, measured range 52.36 – 118.14°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.55716 - 1642.54/(233.386\text{C} + t/^{\circ}\text{C})$; temp range 52 – 118°C (ebulliometry, McDonald et al. 1959)

2105 (calculated by formula, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.18807 - 1416.7/(211 + t/^{\circ}\text{C})$, temp range 36 – 170°C , (Antoine eq. for liquid state, Dreisbach 1961)

2030 (Hoy 1970)

$\log(P/\text{mmHg}) = [-0.2185 \times 9963.9/(T/\text{K})] + 8.50200$; temp range -35 to 10°C (Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9486.6/(T/\text{K})] + 8.142405$; temp range -17.2 to 312.5°C (Antoine eq., Weast 1972–73)

2079* (ebulliometry, fitted to Antoine eq., measured range 304.065 – 415.041 K , Ambrose et al. 1977)

$\log(P/\text{kPa}) = 6.66686 - 1633.288/[(T/\text{K}) - 40.626]$; temp range 351.347 – 415.041 K (Antoine eq.-I, ebulliometry, Ambrose et al. 1977)

- $\log (P/\text{kPa}) = 6.59795 - 1587.182/\{(T/\text{K}) - 45.392\}$; temp range 304.065–415.041 K (Antoine eq.-II, ebulliometry, Ambrose et al. 1977)
 1520, 2666 (20°C, 30°C, Verschuereen 1983)
 2088 (extrapolated average-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.5039 - 1527.764/(221.742 + t/^\circ\text{C})$, temp range 29.8–126.45°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.72515 - 1670.427/(236.091 + t/^\circ\text{C})$, temp range 52.36–118.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 2050 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.38782 - 1533.313/(222.309 + t/^\circ\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 2079 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.66686 - 1633.288/(232.885 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 2076 (comparative ebulliometry data, Ambrose & Ghassee 1987)
 $\ln (P/\text{kPa}) = 15.19234 - 3654.622/[(T/\text{K}) - 45.392]$ (Antoine eq. Ambrose & Ghassee 1987)
 2114 (calculated-Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 7.672 - 2177/(T/\text{K})$, temp range: 238–283 K, (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 9.9268 - 2847/(T/\text{K})$; temp range 243–289 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.68206 - 1642.54/(-39.764 + T/\text{K})$; temp range 289–392 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.39226 - 2258.22/(2762 + T/\text{K})$; temp range 391–550 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5729 - 1572.32/(-46.777 + T/\text{K})$; temp range 290–396 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.82561 - 1748.572/(-28.259 + T/\text{K})$; temp range 391–447 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.22638 - 2010.805/(12.244 + T/\text{K})$; temp range 437–535 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.44129 - 3628.409/(182.674 + T/\text{K})$; temp range 525–593 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)
 1520, 32660 (measured, calculated-solvatochromic parameters., Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 28.3756 - 2.9734 \times 10^3/(T/\text{K}) - 7.032 \cdot \log (T/\text{K}) - 1.5051 \times 10^{-9} \cdot (T/\text{K}) + 2.1806 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 290–593 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$) at 25°C and reported temperature dependence equations):

- 0.0303 (partial pressure, Butler & Ramchandani 1935)
 0.0305 (exptl., Hine & Mookerjee 1975)
 0.0300, 0.0280 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.0115 (calculated, Keene & Galloway 1986)
 0.0101 (effective Henry's law constant, pH 4, Gaffney et al. 1987)
 0.0254 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.121 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0101, 1.01×10^{-4} (at pH 4, pH 7, Howard 1990)
 0.0109, 0.00905, 0.0158 (23°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)
 0.0184 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -25.67 + 8322/(T/\text{K})$, temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0285 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.0431 (calculated-molecular structure, Russell et al. 1992)
 0.0182 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.0115–0.0195 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0245, 0.0145 (counter-flow packed column technique-ion chromatography; "best" exptl value, Johnson et al. 1996)

$\ln [K_H/(M/atm)] = -12.5 + 6200/(T/K)$, temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)

0.0130 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0154 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.650 - 2596/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

-0.30 (shake flask-titration, Leonard et al. 1948)

-0.31 (shake flask-titration, Collander 1951)

-0.29; -0.17 (calculated-fragment const.; calculated- π const., Rekker 1977)

-0.29 (shake flask-radiochemical method, pH 1, Wolfenden 1978)

-0.17, -0.31 (Hansch & Leo 1979)

-0.17 (shake flask, Log P Database, Hansch & Leo 1987)

-0.17 (recommended, Sangster 1989, 1993)

-0.17 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

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

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

no detectable sorption (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

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

-0.21 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

0.00 (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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (0.6 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 26.7 \text{ d}$ for the vapor-phase reaction with 5×10^5 hydroxyl radical/cm³ in air at 25°C (flash photolysis-resonance fluorescence technique, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k(aq.) \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water; $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2.0–5.5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (7.4 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-resonance fluorescence, Dagaut et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air, and $k(soln) = 2.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}(calc) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996).

Hydrolysis:

Biodegradation: > 90% degradation in 3 d using an activated sludge inoculum; in 24 h in batch aeration in sewage and 14 d using sediment from the Rhine river as inocula (Howard 1990).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 26.7 \text{ d}$, based on measured rate constant of $0.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/cm³ in air at 25°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{1/2} = 26\text{--}46 \text{ yr}$, based on OH radical concn. in sunlit natural water of $1 \times 10^{-17} \text{ mol/L}$ (Howard 1990).

Groundwater:

Sediment: > 90% degradation in 14 d using Rhine River sediment as inocula (Kool 1984; quoted, Howard 1990).

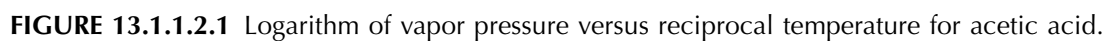
Soil:

Biota:

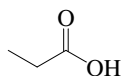
TABLE 13.1.1.2.1

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

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Potter & Ritter 1954		McDonald et al. 1959	
summary of literature data		ebulliometry		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−17.2	133	55.75	10114	29.8	2666	52.36	8297
6.3	666.6	66.07	16500	40.25	4693	55.63	9998
17.5	1333	91.13	42066	51.08	8013	67.20	16517
29.9	2666	117.72	101325	55.54	9866	91.49	42302
43	5333			60.93	12599	105.49	68210
51.7	7999	bp/°C	100.79	65.50	15332	115.51	94156
63	13332			71.04	19345	116.83	98175
80	26664			75.70	23105	117.27	99584
99	53329			80.41	28038	117.71	110901
118.1	101325			85.69	34224	118.14	102318
				90.59	40930		
mp/°C	16.7			95.66	48982	eq. 2	P/mmHg
				100.29	57488	A	7.55716
				105.45	68314	B	1642.54
				110.0	79193	C	233.386
				115.12	92992		
				118.41	102978	mp/°C	16.34
				122.44	116137		
				123.86	121256		
				126.45	130669		
				Antoine eq.			
				eq. 2	P/mmHg		
				A	7.4275		
				B	1558.03		
				C	224.79		



13.1.1.3 Propionic acid



Common Name: Propionic acid

Synonym: methylacetic acid, propanoic acid

Chemical Name: propanoic acid, propionic acid

CAS Registry No: 79-09-4

Molecular Formula: $C_3H_6O_2$, CH_3CH_2COOH

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

−20.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.99336, 0.98797 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9930 (Weast 1982–83)

Molar Volume (cm^3/mol):

74.6 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

−6.80 (pK value, Perrin 1972)

4.874 (Dean 1985; Riddick et al. 1986)

4.870 (Sangster 1989)

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

10.66 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

550* (interpolated-regression of tabulated data, temp range 4.6 – $141.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.92234 - 1869.4/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

7605* ($72.39^{\circ}C$, ebulliometry, measured range 72.39 – $140.80^{\circ}C$, Dreisbach & Shrader 1949)

446 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.35027 - 1497.775/(194.12 + t/^{\circ}C)$, temp range 60 – $185^{\circ}C$ (Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 12454.4/(T/K)] + 9.647835$; temp range 4.6 – $238^{\circ}C$ (Antoine eq., Weast 1972–73)

435* (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.64344 - 1594.723/[(T/K) - 70.545]$; temp range 328 – $438\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

500, 442 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.84202 - 1736.007/(218.032 + t/^{\circ}C)$, temp range 72.39 – $128.34^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67457 - 1615.227/(204.788 + t/^{\circ}C)$, temp range 55.11 – $164.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

257 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.403 - 950.2/(130.3 + t/^{\circ}C)$, temp range 56 – $139.5^{\circ}C$ (Antoine eq., Dean 1985, 1992)

451 (Riddick et al. 1986)

$\log(P/kPa) = 6.64334 - 1594.273/(202.605 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

452 (comparative ebulliometry, Ambrose & Ghiassee 1987)

$\ln (P/\text{kPa}) = 15.29686 - 3670.949/[(T/\text{K}) - 70.545]$, (Antoine eq., Ambrose & Ghasseer 1987)

$\log (P_L/\text{kPa}) = 6.60267 - 1577.96/(-79.844 + T/\text{K})$, temp range 343–419 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 9.24101 - 12835.99/(-23.07 + T/\text{K})$, temp range 414–511 K (Antoine eq.-II, Stephenson & Malanowski 1987)

453, 8758 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 20.2835 - 3.1165 \times 10^3/(T/\text{K}) - 3.6015 \cdot \log (T/\text{K}) - 1.3892 \times 10^{-3} \cdot (T/\text{K}) + 7.1801 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 252–604 K (vapor pressure eq., Yaws 1994)

14560* (88.37°C, VLE still-manometry, measured range 88.37–140.59°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 18.105654 - 5640.3443/[(t/^\circ\text{C}) + 277.46143]$; temp range 88.37–140.59°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.0445 (partial pressure, Butler & Ramchandani 1935)

0.0450 (exptl., Hine & Mookerjee 1975)

0.0420, 0.0430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.0298 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

0.0163, 0.00151, 0.0289 (23.1°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)

0.0180 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0431 (calculated-bond contribution, Brimblecombe et al. 1992)

0.0177 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

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

0.25 (shake flask-titration, Collander 1951)

0.23, 0.24 (calculated- π const., calculated-fragment const., Rekker 1977)

0.33, 0.25 (Hansch & Leo 1979)

0.27 (shake flask-titration, Umland 1983)

0.33 (recommended, Sangster 1989; 1994)

0.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.6 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k = 2.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 4.0 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k = (1 \pm 0.5) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (1.22 \pm 0.12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{OH} = 1.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = (1.22 - 1.60) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 13.1.1.3.1

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

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)		ln P = A – B/(C + T/K)		(3a)	
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981		Clifford et al. 2004	
summary of literature data		ebulliometry		comparative ebulliometry		VLE still-Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
4.60	133.3	72.39	7605	55.174	2891	88.37	14560
28.0	666.6	76.75	8851	57.414	3274	95.22	19580
39.7	1333	79.68	10114	60.143	3787	105.80	29650
52.0	2666	90.73	16500	63.850	4594	113.59	39730
65.8	5333	114.62	42066	67.094	5417	119.78	49790
74.1	7999	128.34	67661	70.860	6529	125.94	59860
85.8	13332	140.80	101325	74.311	7713	129.50	69920
102.5	26664			78.096	9217	133.65	79990
122.0	53329			81.787	10917	137.18	90070
141.5	101325			85.630	12961	138.82	95100
				89.553	15372	140.59	101210
mp/°C	–22			93.303	18022		
				98.207	22058	Antoine eq.	
				102.401	26085	eq. 3a	P/kPa
				107.174	31400	A	18.105654
				111.847	37437	B	56403343
				116.747	44780	C	277.46143
				122.130	54180		
				126.788	63579	data also fitted to Wagner eq.	
				131.723	74946		
				137.045	89022		
				141.105	101143		
				25.0	451		
				eq. 3	P/kPa		
				A	6.64334		
				B	1594.273		
				C	–70.545		
				data also fitted to Chebyshev and Wagner equations			
				bp/K	436.868		

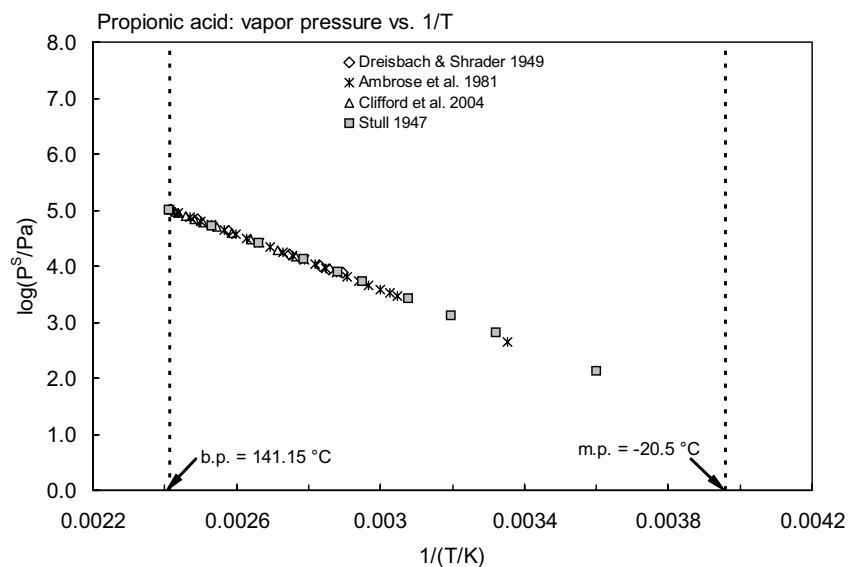
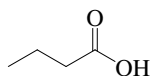


FIGURE 13.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propionic acid.

13.1.1.4 Butyric acid



Common Name: Butyric acid

Synonym: butanoic acid, *n*-butyric acid, ethylacetic acid

Chemical Name: *n*-butyric acid, butyric acid

CAS Registry No: 107-92-6

Molecular Formula: $C_4H_8O_2$, $CH_3CH_2CH_2COOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−5.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

163.75 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.95767, 0.95273 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9582 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.0 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

4.817 (Dean 1985)

4.822 (Riddick et al. 1986)

4.820 (Sangster 1993)

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

11.6 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($25.5^{\circ}C$, temp range 25.5 – $163.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 8.19524 - 2089.9/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

4716* ($90.92^{\circ}C$, ebulliometry, measured range 90.92 – $163.25^{\circ}C$, Dreisbach & Shrader 1949)

95.77 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.38423 - 1542.6/(179.0 + t/^{\circ}C)$, temp range 82 – $210^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11881.2/(T/K)] + 8.773450$; temp range 25.5 – $352^{\circ}C$ (Antoine eq., Weast 1972–73)

83.95* (comparative ebulliometry, fitted to Antoine eq., measured range 340 – $452 K$, Ambrose et al. 1981)

$\log(P/kPa) = 6.55643 - 1563.444/[(T/K) - 93.307]$; temp range 339.7 – $452 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

104, 92 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.8682 - 1766.906/(200.097 + t/^{\circ}C)$, temp range 90.2 – $163.25^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67596 - 1642.683/(188.013 + t/^{\circ}C)$; temp range 76.53 – $178.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

104.3 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.7399 - 1764.7/(199.9 + t/^{\circ}C)$; temp range 90 – $163^{\circ}C$ (Antoine eq., Dean 1985, 1992)

102.0 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.55643 - 1563.444/(179.843 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

- 101 (comparative ebulliometry, Ambrose & Ghiassee 1987)
 $\ln(P/\text{kPa}) = 15.09674 - 3599.963/[(T/\text{K}) - 93.307]$, (Antoine eq. from previous comparative ebulliometry measurements, Ambrose & Ghiassee 1987)
 $\log(P_L/\text{kPa}) = 6.50913 - 1542.6/(-94.15 + T/\text{K})$; temp range 355–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.3554 - 2180.05/(-29.337 + T/\text{K})$; temp range 437–592 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 11.53324 - 5291.631/(128.778 + T/\text{K})$; temp range 301–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 8.0847 - 3.3219 \times 10^3/(T/\text{K}) + 2.4312 \cdot \log(T/\text{K}) - 1.1734 \times 10^{-2} \cdot (T/\text{K}) + 5.7992 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–628 K (vapor pressure eq., Yaws 1994)
 14560* (110.4°C, VLE still-manometry, measured range 110.4–162.9°C, Clifford et al. 2004)
 $\ln(P/\text{kPa}) = 14.511627 - 3164.4707/[(t/^\circ\text{C}) + 156.56122]$; temp range 110.4–162.9°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0542 (partial pressure, Butler & Ramchandani 1935)
 0.0542; 0.0590; 0.0650 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 0.0375 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.0222 (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0654 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.358 (calculated-molecular structure, Russell et al. 1992)
 0.0211 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

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

- 0.79 (shake flask-TN, Collander 1951)
 0.94 (calculated-TSA, Iwase et al. 1985)
 0.824, 0.70 (calculated-CLOGP, calculated-M.O., Bodor et al. 1989)
 0.79 (recommended, Sangster 1993)
 0.79 (recommended, 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.4 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K was determined using (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985, 1989)

$k(\text{apparent}) \leq 4 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–4 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH} = 1.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 3.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH}(\text{calc}) = 3.11 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.1.4.1

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

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)	ln P = A – B/(C + T/K)		(3a)		
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981	Clifford et al. 2004		
summary of literature data		ebulliometry		comparative ebulliometry	VLE still-manometry		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.5	133.3	90.92	4716	76.524	2939	110.4	14560
49.8	666.6	95.01	5704	78.773	3305	117.72	19580
61.5	1333	98.35	6639	81.494	3818	128.17	29650
74.0	2666	101.32	7586	85.202	4614	135.85	39720
88.0	5333	112.57	16500	88.517	5443	141.84	40790
95.5	7999	136.57	42066	92.350	6558	147.07	59860
108.0	13332	150.70	67661	95.880	7754	151.66	69920
125.5	26664	163.25	101326	99.708	9255	155.81	79990
144.5	53329			103.451	10955	159.46	90070
163.5	101325			107.241	13000	161.36	95100
				111.319	15409	162.90	100040
mp/°C	–4.70			115.124	18601		
				120.102	22098	Antoine eq.	
				124.357	26126	eq. 3a	P/kPa
				129.207	31448	A	14.511627
				133.944	37489	B	3164.4707
				144.392	54256	C	156.56122
				149.125	63651		
				154.135	75000	data also fitted to Wagner eq.	
				159.367	89123		
				163.687	101252		
				164.110	102558		
				164.553	103927		
				169.357	120015		
				173.698	136172		
				178.873	157694		
				Antoine eq.			
				eq. 3	P/kPa		
				A	6.55643		
				B	1563.444		
				C	–1563.444		
				data also fitted to Chebyshev and Wagner equations			

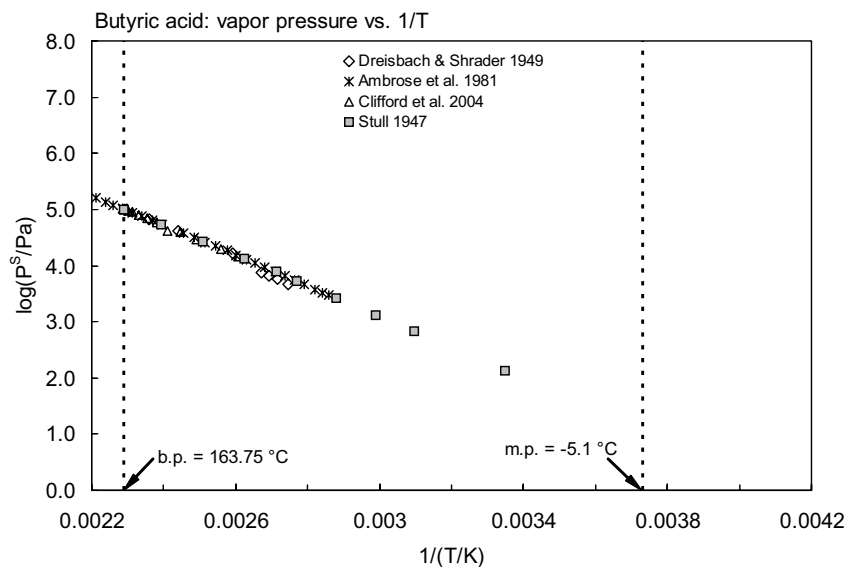
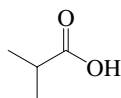


FIGURE 13.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for butyric acid.

13.1.1.5 Isobutyric acid



Common Name: Isobutyric acid

Synonym: isobutanoic acid, *i*-butyric acid, 1-butyric acid, dimethylacetic acid, 2-methylpropionic acid, isopropylformic acid

Chemical Name: *i*-butyric acid, isobutyric acid

CAS Registry No: 79-31-2

Molecular Formula: $C_4H_8O_2$, $(CH_3)_2CHCOOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−46.0 (Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

154.45 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9490 (Verschuereen 1983)

0.9682 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.860 (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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

228000 ($20^{\circ}C$, synthetic method, Jones 1929)

200000 ($20^{\circ}C$, quoted, Verschuereen 1983)

170000 (Dean 1985)

228000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

273.8* (interpolated-regression of tabulated data, temp range 14.7 – $154.5^{\circ}C$, Stull 1947)

185 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.40246 - 1529.2/(185.0 + t/^{\circ}C)$, temp range 73 – $190^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11182.8/(T/K)] + 8.55228$; temp range 14.7 – $336^{\circ}C$ (Antoine eq., Weast 1972–73)

185.0 (Riddick et al. 1986)

184* (comparative ebulliometry, measured range 344.3 – $445.6 K$, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.31143 - 3695.332/[(T/K) - 82.0]$; temp range 344.3 – $447 K$ (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)

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

$\log(P_L/kPa) = 7.20794 - 2023.52/(-38.649 + T/K)$; temp range 288 – $428 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.11635 - 2006.61/(-35.297 + T/K)$, temp range 428 – $562 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 11.3037 - 3.1625 \times 10^3/(T/K) + 0.7263 \cdot \log(T/K) - 8.9331 \times 10^{-3} \cdot (T/K) + 4.8215 \times 10^{-6} \cdot (T/K)^2$; temp range 227 – $609 K$ (vapor pressure eq., Yaws 1994)

14550* ($102.6^{\circ}C$, VLE still-manometer, measured range 102.6 – $153.01^{\circ}C$, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 15.176238 - 3527.8614/[(t/^{\circ}\text{C}) + 180.5140]$; temp range 102–153.01 $^{\circ}\text{C}$ (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$ or as indicated):

0.0178, 0.0289, 0.0633 (23.7 $^{\circ}\text{C}$, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)

0.0897 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0899 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

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

0.50, 1.13 (calculated, Verschuereen 1983)

0.94 (recommended, Sangster 1993)

1.10 (at pH 3.5, quoted, Hansch et al. 1995)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}^* = (2.0 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988; Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 13.1.1.5.1

Reported vapor pressures of isobutyric acid (2-methyl propanoic acid) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(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)			
Stull 1947		Ambrose & Giassee 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa	$t/^{\circ}\text{C}$	P/Pa
14.7	133.3	344.287	3425	102.06	14550
39.3	666.6	347.850	4128	108.99	18580
51.2	1333	350.797	4801	118.62	29650
64.0	2666	355.776	6153	126.28	39720
77.8	5333	357.992	6852	132.29	49790
86.3	7999	360.006	7548	137.60	59850
98.0	13332	361.903	8260	142.36	69920
115.8	26664	365.785	9886	146.62	79990

TABLE 13.1.1.5.1 (Continued)

Stull 1947		Ambrose & Ghiasee 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
134.5	53329	369.394	11370	150.21	90070
154.5	101325	375.207	15006	151.71	95100
mp/°C	−47	380.090	18440	153.01	100590
		384.218	21842	Antoine eq. eq. 3(a)	P/kPa
		387.840	25241		
		392.544	30312		
		399.095	38759		
		405.577	48959		
		409.363	55877	A	15.176238
		412.692	62629	B	3527.8614
		↓	↓	C	180.5140
		445.602	172068	data also fitted to Wagner eq.	
		298.15	184		
Antoine eq.					
eq. 3(a)		P/kPa			
A		15.31143			
B		3695.332			
C		−82.0			
bp/K		427.57			
data also fitted to Wagner eq.					

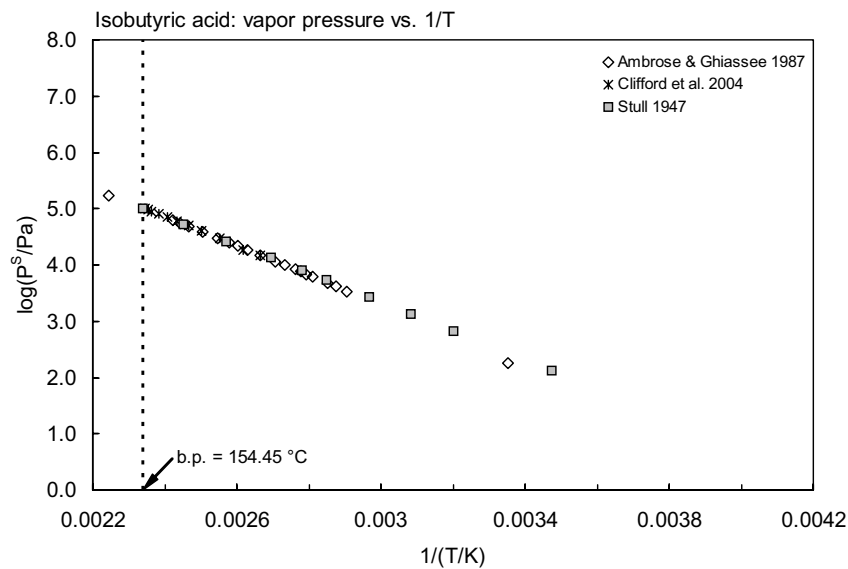
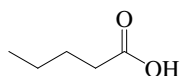


FIGURE 13.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for isobutyric acid.

13.1.1.6 *n*-Valeric acid

Common Name: *n*-Valeric acid

Synonym: pentanoic acid, valeric acid

Chemical Name: *n*-valeric acid, valeric acid

CAS Registry No: 109-52-4

Molecular Formula: $C_5H_{10}O_2$, $CH_3CH_2CH_2CH_2COOH$

Molecular Weight: 102.132

Melting Point ($^{\circ}C$):

−33.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

186.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9391 (Weast 1982–83)

0.9390 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.820 ($18^{\circ}C$, Weast 1982–83)

4.860 (Riddick et al. 1986)

4.830 (Sangster 1989, 1993)

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

14.17 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 1.0$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

26000 ($20^{\circ}C$, quoted, Amidon et al. 1975)

24000 (Verschuereen 1983; Dean 1985)

24000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.6* (extrapolated-regression of tabulated data, temp range 42.2 – $184.4^{\circ}C$, Stull 1947)

18.75 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.57366 - 1694.37/(175.0 + t/^{\circ}C)$, temp range 102 – $250^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 13370.3/(T/K)] + 9.271178$; temp range 42.2 – $184.4^{\circ}C$ (Antoine eq., Weast 1972–73)

20.0 ($20^{\circ}C$, Verschuereen 1983)

4.33, 6.37 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 4.58366 - 609.613/(62.754 + t/^{\circ}C)$; temp range 72.4 – $173.7^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.0835 - 878.669/(95.711 + t/^{\circ}C)$; temp range 81.1 – $116.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 5.412 - 591/(60 + t/^{\circ}C)$; temp range 72 – $174^{\circ}C$ (Antoine eq., Dean 1985, 1992)

19.0 (Riddick et al. 1986)

$\log(P/kPa) = 6.7818 - 1777.2/(186.6 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

21.0* (comparative ebulliometry, measured range 372.5 – $465.3\ K$, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.25555 - 3811.202/[(T/K) - 101.0]$, temp range 372.5 – $456.3\ K$ (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)

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

$\log (P_L/\text{kPa}) = 6.69856 - 1694.37/(-98.15 + T/\text{K})$, temp range 375–523 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 15.3454 - 3.9024 \times 10^3/(T/\text{K}) - 0.024353 \cdot \log (T/\text{K}) - 1.1099 \times 10^{-2} \cdot (T/\text{K}) + 5.6315 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 239–651 K (vapor pressure eq., Yaws 1994)

14560 (130°C, VLE still-manometer, measured range 130–178.77°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 36.410366 - 30029.229/(t/^\circ\text{C}) + 760.44819$; temp range 130–178.77°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.0478 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -15.37 + 6879/(T/\text{K})$; temp range 278.15–308.15 K. (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0618, 0.0989 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0448* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -14.3371 + 6582.96/(T/\text{K})$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0310 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.030 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.861 - 2865/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.42 (Scherrer & Howard 1979)

0.99, 1.69 (calculated, Verschueren 1983)

1.39 (recommended, Sangster 1993)

1.39 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

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

Half-Lives in the Environment:

TABLE 13.1.1.6.1

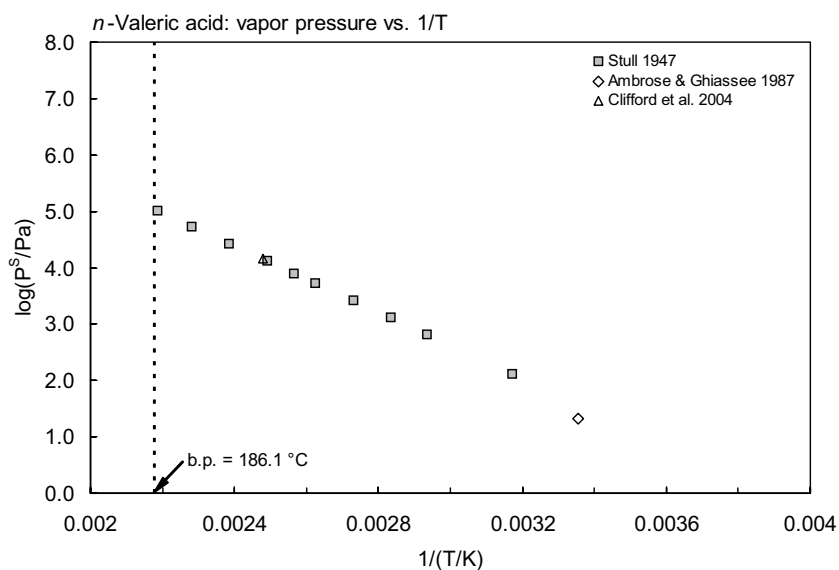
Reported vapor pressures and Henry's law constants of n-valeric acid at various temperatures

$\log P = A - B/(T/K)$	(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)						
Vapor pressure				Henry's law constant			
Stull 1947		Ambrose & Ghiassaei 1987		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping	
t/^{\circ}C	P/Pa	T/K	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	H/(Pa m^3/mol)
42.2	133.3	372.543	3410	130.0	14560	5	0.00823
67.7	666.6	376.278	4112	137.56	19590	15	0.018
79.8	1333	379.415	4801	143.92	24630	25	0.0448
93.1	2666	384.489	6125	149.04	29650	35	0.0878

(Continued)

TABLE 13.1.1.6.1 (Continued)

Vapor pressure						Henry's law constant	
Stull 1947		Ambrose & Gdiassee 1987		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
116.6	7999	398.670	11637	163.33	49780	ln H = A - B/(T/K)	
128.3	13332	404.759	15006	168.74	59850	H/(mol kg ⁻¹)	
146.0	26664	414.079	21807	173.30	69920	A	-14.3371
165.0	53329	422.753	30285	175.33	74960	B	6582.96
184.4	101325	429.637	55786	17720	79990		
		443.796	62659	17877	86030		
mp/°C	-34.5	449.980	76308				
		454.060	86528	Antoine eq.			
		460.052	101592	eq. 2a	P/Pa		
		405.378	120678	A	36.410366		
				B	30029.229		
				C	760.44819		
		Antoine eq.					
		eq. 2a	P/kPa				
		A	15.2555	data also fitted to Wagner eq.			
		B	3811.202				
		C	-101.0				
		data also fitted to Wagner eq.					

FIGURE 13.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-valeric acid.

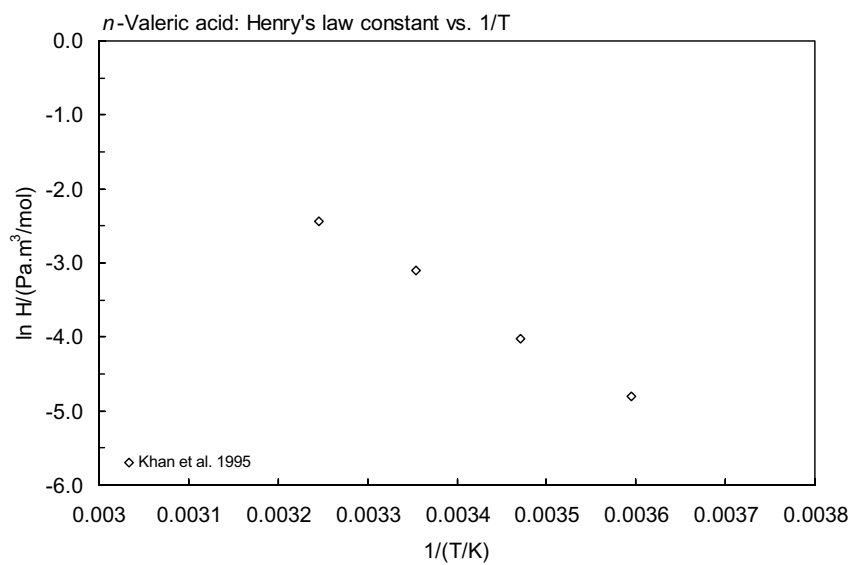
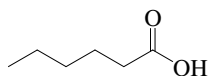


FIGURE 13.1.1.6.2 Logarithm of Henry's law constant versus reciprocal temperature for *n*-valeric acid.

13.1.1.7 Hexanoic acid (Caproic acid)



Common Name: Hexanoic acid

Synonym: butylacetic acid, caproic acid, *n*-hexanoic acid

Chemical Name: butylacetic acid, hexanoic acid, *n*-hexanoic acid

CAS Registry No: 142-62-1

Molecular Formula: $C_6H_{12}O_2$, $CH_3(CH_2)_4COOH$

Molecular Weight: 116.158

Melting Point ($^{\circ}C$):

−3 (Lide 2003)

Boiling Point ($^{\circ}C$):

205.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.850 (Dean 1985; Bintein & Devillers 1994)

4.879 (Riddick et al. 1986)

4.870 (Sangster 1989, 1993)

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

15.4 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9887 (Valvani et al. 1981)

11000 (Verschuereen 1983)

10816 (Windholz 1983)

6391 (calculated-activity coefficient γ from UNIFAC, Banerjee 1985)

9580 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($71.4^{\circ}C$, summary of literature data, temp range 71.4 – $202^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 16189.4/(T/K)] + 10.431464$; temp range 71.4 – $202^{\circ}C$ (Antoine eq., Weast 1972–73)

4.40 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.76323 - 1789.425/(T/K) - 101.930$; temp range: 386.3 – $441.8 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

26.7 ($20^{\circ}C$, Verschuereen 1983)

9.92, 1.65 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.74777 - 1779.677/(178.361 + t/^{\circ}C)$, temp range 113.1 – $168.6^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1981, Boublik et al. 1984)

$\log(P/kPa) = 6.06182 - 1347.897/(127.391 + t/^{\circ}C)$, temp range 98.1 – $179.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.9249 - 1340.8/(126.6 + t/^{\circ}C)$, temp range 98 – $179^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5.00 (Riddick et al. 1986)

$\log(P/kPa) = 6.76323 - 1789.425/(171.22 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

6.0 (calculated from Wagner eq. derived from experimental data, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.30352 - 3957.396/[(T/K) - 108]$ (Antoine eq., Ambrose & Ghassee 1987)

$\log(P_L/kPa) = 7.08241 - 2009.93/(-82.69 + T/K)$; temp range 335 – $487 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 55.7058 - 5.6602 \times 10^3/(T/K) - 15.458 \cdot \log (T/K) + 1.0823 \times 10^{-9} \cdot (T/K) + 1.8718 \times 10^{-13} \cdot (T/K)^2$;
temp range 270–667 K (vapor pressure eq., Yaws 1994)

9520 (140.25°C, VLE still-manometer, measured range 140.25–178.28°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 13.46595 - 2642.198/[t/^\circ\text{C} + 95.20133]$; temp range 140.25–178.28°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

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

0.0768 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -12.69 + 5988/(T/K)$; temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0873, 0.149 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0720* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -13.9424 + 6303.73/(T/K)$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0583 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0556 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.955 - 2520/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.88 (Scherrer & Howard 1979)

1.87 (HPLC-RT correlation, D'Amboise & Hanai 1982)

1.92 (shake flask-titration, Umland 1983)

2.09 (shake flask-fluorescence, Nishimura et al. 1985)

1.32 (calculated-activity coefficient γ from UNIFAC, Banerjee & Howard 1988)

2.03 ± 0.01 (potentiometric titration, Hersey et al. 1989)

1.92 (recommended, Sangster 1989, 1993)

1.92 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

1.38; 1.42; 1.57 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)

1.46; 0.88 (soil, quoted exptl.; calculated-MCI χ and fragment contribution, Meylan et al. 1992)

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

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

Half-Lives in the Environment:

TABLE 13.1.1.7.1
Reported vapor pressures and Henry’s law constants of hexanoic acid (caproic acid) at various temperatures

Vapor pressure						Henry’s law constant	
Stull 1947		Ambrose et al. 1981		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometer		gas stripping	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
71.4	133.3	386.270	2952	140.25	9520	5	0.0167
89.5	666.6	388.571	3314	149.73	14560	15	0.036
99.5	1333	391.485	3831	156.77	19590	25	0.072
111.8	2666	395.428	4638	162.47	24630	35	0.150
125.0	5333	398.865	5459	166.88	29640		
133.3	7999	402.913	6576	171.11	34680	ln H = A – B/(T/K)	
144.0	13332	406.610	7762	174.73	39720		H/(mol kg ⁻¹)
160.8	26664	410.665	9267	178.28	44750	A	–13.9424
181.0	53329	414.581	10963			B	6303.73
202.0	101325	418.705	13001	Antoine eq.			
		422.887	15422	eq. 2a	P/Pa		
mp/°C	–1.5	432.157	22112	A	13.46595		
		441.779	31458	B	2642.198		
				C	95.20133		
		eq. 2	P/kPa				
		A	6.76323	data also fitted to Wagner eq.			
		B	1789.425				
		C	–101.930				
data also fitted to Wagner eq.							

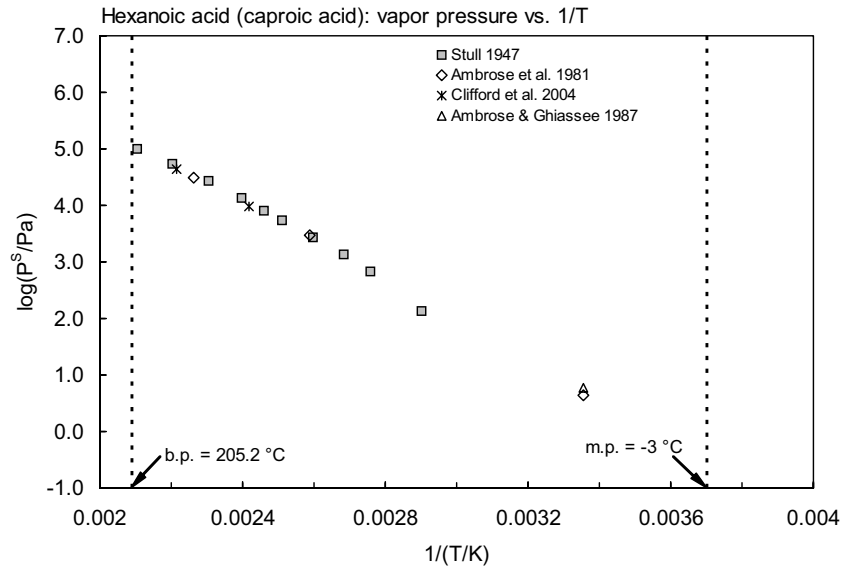


FIGURE 13.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for hexanoic acid.

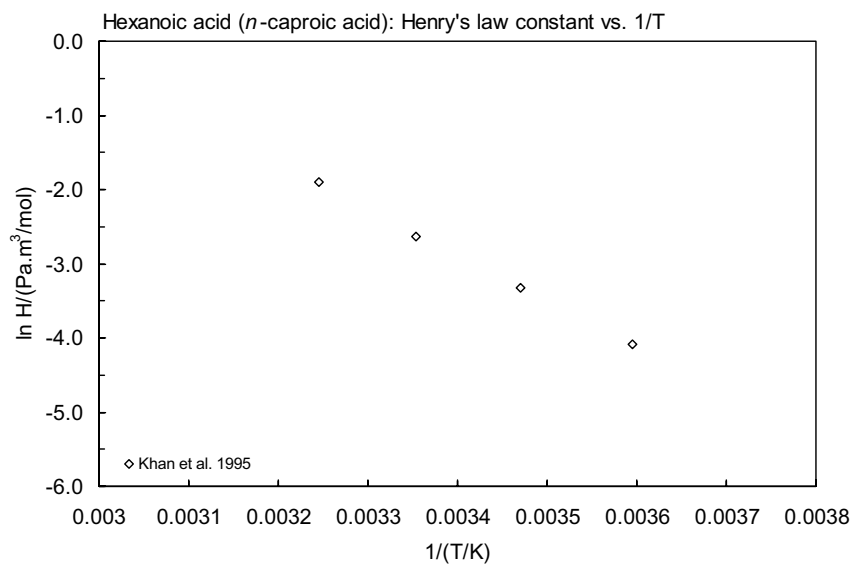
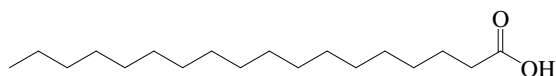


FIGURE 13.1.1.7.2 Logarithm of Henry's law constant versus reciprocal temperature for hexanoic acid.

13.1.1.8 Stearic acid (Octadecanoic acid)



Common Name: Stearic acid

Synonym: octadecanoic acid

Chemical Name: stearic acid, octadecanoic acid, *n*-octadecylic acid

CAS Registry No: 57-11-4

Molecular Formula: $C_{18}H_{36}O_2$, $CH_3(CH_2)_{16}COOH$

Molecular Weight: 284.478

Melting Point ($^{\circ}C$):

69.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

350 (dec., Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9408 (Weast 1982–83)

Molar Volume (cm^3/mol):

335.9 ($70^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.50 (estimated, Sangster 1989)

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

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

39.57; 43.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.368 (mp at $69.3^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

340 (Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133.3 ($173.7^{\circ}C$, summary of literature data, temp range: 173.7 – $370^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 19306.6/(T/K)] + 9.457471$; temp range: 173.7 – $370^{\circ}C$, (Antoine eq., Weast 1972–73)

1.69×10^{-12} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17126 - 2157.5/(-153.78 + T/K)$; temp range 349–415 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.85188 - 1717.93/(-201.829 + T/K)$; temp range 447–649 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -40.3638 - 4.7724 \times 10^3/(T/K) + 24.502 \cdot \log(T/K) - 3.7665 \times 10^{-2} \cdot (T/K) + 1.4595 \times 10^{-5} \cdot (T/K)^2$; temp range 343–799 K (vapor pressure eq., Yaws 1994)

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

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

8.23 (HPLC-RT correlation, D'Amboise & Hanai 1982)

8.23 (recommended, Sangster 1989, 1993)

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

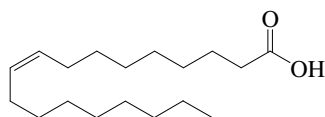
Bioconcentration Factor, $\log BCF$:

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

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

Half-Lives in the Environment:

13.1.1.9 Oleic acid



Common Name: Oleic acid

Synonym: *cis*-9-octadecenoic acid, (*Z*)-9-octadecenoic acid

Chemical Name: oleic acid

CAS Registry No: 112-80-1

Molecular Formula: $C_{18}H_{34}O_2$, $CH_3(CH_2)_7CH=CH(CH_2)_6CH_2COOH$

Molecular Weight: 282.462

Melting Point ($^{\circ}C$):

13.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

360 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8870 ($25^{\circ}C$, Riddick et al. 1986)

0.8935 (Lide 2003)

Molar Volume (cm^3/mol):

314.7 (Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

5.02 (Riddick et al. 1986)

4.50 (Sangster 1989)

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

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

insoluble (McBain & Richards 1946; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133 ($178.5^{\circ}C$, summary of literature data, temp range 176.5 – $360^{\circ}C$, Stull 1947)

0.00144 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 20326.7/(T/K)] + 9.930301$; temp range 176.5 – $360^{\circ}C$ (Antoine eq., Weast 1972–73)

0.00113 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.22018 - 3711.59/(-36.125 + T/K)$; temp range 444 – $635\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 78.6973 - 8.8227 \times 10^3/(T/K) - 22.472 \cdot \log(T/K) + 4.8353 \times 10^{-11} \cdot (T/K) + 2.6578 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – $633\ K$ (vapor pressure eq., Yaws 1994)

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

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

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

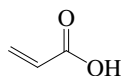
7.64 (recommended, Sangster 1989, 1993)

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

Bioconcentration Factor, $\log BCF$:

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

13.1.1.10 Acrylic acid (2-Propenoic acid)



Common Name: Acrylic acid

Synonym: acroleic acid, ethylenecarboxylic acid, 2-propenoic acid, propenoic acid

Chemical Name: acrylic acid, 2-propenoic acid, propenoic acid

CAS Registry No: 79-10-7

Molecular Formula: $C_3H_4O_2$, $CH_2=CHCOOH$

Molecular Weight: 72.063

Melting Point ($^{\circ}C$):

12.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141 (Lide 1003)

Density (g/cm^3 at $20^{\circ}C$):

1.0511 (Weast 1982–83; Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.9 (calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

–4.41 (Perrin 1972)

4.25 (pK_a , Weast 1982–83)

4.26 (pK_a , Dean 1985)

4.255 (pK_a , Riddick et al. 1986)

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

11.13 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

570.8 (interpolated-regression of tabulated data, temp range 3.5 – $141^{\circ}C$, Stull 1947)

506.5 (Hoy 1970)

570 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 10955.1/(T/K)] + 8.659704$; temp range 3.5 – $141^{\circ}C$ (Antoine eq., Weast 1972–73)

426.6 ($20^{\circ}C$, Verschueren 1983)

$\log(P/mmHg) = 5.65204 - 648.629/(154.683 + t/^{\circ}C)$; temp range 20 – $70^{\circ}C$ (Antoine eq., Dean 1985, 1992)

533.0 (Howard et al. 1986)

1030 ($20^{\circ}C$, Riddick et al. 1986)

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

$\log(P_L/kPa) = 6.93296 - 1827.9/(-43.15 + T/K)$; temp range 341 – $414\ K$ (Antoine eq., Stephenson & Malanowski 1987)

533, 12530 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 23.0607 - 3.1347 \times 10^3/(T/K) - 4.8813 \cdot \log(T/K) + 4.369 \times 10^{-4} \cdot (T/K) - 4.9161 \times 10^{-13} \cdot (T/K)^2$; temp range 287 – $615\ K$ (vapor pressure eq., Yaws 1994)

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

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

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

- 0.43 (Leo et al. 1971)
- 0.31, 0.43 (calculated, Verschueren 1983)
- 0.35 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} t_{1/2} = 2.5\text{--}23.8$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous screening test data (Dore et al. 1975; Sasaki 1978; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic reactor test data (Chou et al. 1979; selected, Howard et al. 1991)
 $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.5\text{--}23.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

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

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

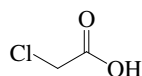
Groundwater: $t_{1/2} = 48\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

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

Biota:

13.1.1.11 Chloroacetic acid



Common Name: Chloroacetic acid

Synonym:

Chemical Name: chloroacetic acid (α or β)

CAS Registry No: 79-11-8

Molecular Formula: $\text{C}_2\text{H}_3\text{ClO}_2$, ClCH_2COOH

Molecular Weight: 94.497

Melting Point ($^\circ\text{C}$):

61.2 (α , Stull 1947; Yalkowsky & Valvani 1980)

56.0 (β , Yalkowsky & Valvani 1980)

56–63 (Weast 1982–83; Dean 1985)

63 (Lide 2003)

Boiling Point ($^\circ\text{C}$):

189.3 (Lide 2003)

Density (g/cm^3 at 20°C):

1.4043 (40°C , Weast 1982–83)

Molar Volume (cm^3/mol):

68.8 (63°C , Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

2.85 (Weast 1982–83)

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

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

56 (estimated, Yalkowsky & Valvani 1980)

36.73, 42.22 (observed for α , observed for β , Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.424 (mp at 63°C)

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

120835 (α , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

107200 (β , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

109000 (shake flask-titrimetric assay, Bowden et al. 1998)

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

39.70* (extrapolated-regression of tabulated data, temp range 43.0 – 189.5°C , Stull 1947)

$\log (P/\text{mmHg}) = 8.28534 - 2263.7/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

6301* (112.8°C , ebulliometry, measured range 112.8 – 187.55°C , Dreisbach & Shrader 1949)

4141* (104.47°C , ebulliometry, measured range 104.47 – 190.27°C , McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.56597 - 1733.96/(180.996 + t/^\circ\text{C})$; temp range: 104 – 190°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log (P/\text{mmHg}) = [-0.2185 \times 13134.5/(T/\text{K})] + 9.099371$; temp range 43 – 189°C (Antoine eq., Weast 1972–73)

18.52, 12.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.67559 - 1723.714/(180.01 + t/^\circ\text{C})$; temp range 104 – 190.27°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.29612 - 1468.443/(154.397 + t/^\circ\text{C})$; temp range 123.19 – 187.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

18.52 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.55016 - 1723.365/(179.98 + t/^\circ\text{C})$; temp range 104 – 190°C (Antoine eq., Dean 1985, 1992)

8.51, 11.5 (extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.69087 - 1733.96/(-92.154 + T/K)$; temp range 336–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.67975 - 1727.293/(-97.742 + T/K)$; temp range 377–464 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 42.6726 - 4.597 \times 10^3/(T/K) - 11.348 \cdot \log (T/K) - 2.8515 \times 10^{-10} \cdot (T/K) + 1.7995 \times 10^{-6} \cdot (T/K)^2$; temp range 333–686 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

0.000938 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1}))] = -21.087 + 9742.6/(T/K)$, temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 7.343 - 4104/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.22 (shake flask, Hansch & Leo 1987; recommended, Hansch et al. 1995)

0.22 (recommended, Sangster 1993)

0.22 (calculated-fragment const. with correction factors in multiCASE program, Dambrosky et al. 2001)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

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

Volatilization:

Photolysis: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991);

atmospheric photolysis $t_{1/2} = 1900\text{--}19000$ h, based on estimated aqueous photolysis half-life (Howard et al. 1991);

photocatalyzed mineralization by the presence of TiO_2 with the rate of 5.5 ppm/min per gram of catalyst (Ollis 1985).

Hydrolysis: first-order hydrolysis $t_{1/2} = 23000$ h, based on losses in dark control tests during photolysis experiments (Draper & Crosby 1983; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on river die-away tests using radio-labeled material (Boethling & Alexander 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

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

Surface water: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991); $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

Sediment:

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

Biota:

TABLE 13.1.1.11.1

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

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & \end{aligned}$$

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959	
summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.0	133	112.8	6301	104.47	4141
68.3	666.6	123.19	10114	114.60	6675
81.0	1333	134.67	16468	128.32	12103
94.2	2666	159.95	42066	146.78	25198
109.2	5333	174.44	67661	167.51	38583
118.3	7999	187.55	101325	187.59	97205
130.7	13332			189.35	102165
140.0	26664			190.27	104738
169.0	53329				
189.5	101325			mp/°C	62.65
mp/°C	61.2			eq. 2	P/mmHg
				A	7.56597
				B	1733.96
				C	180.996

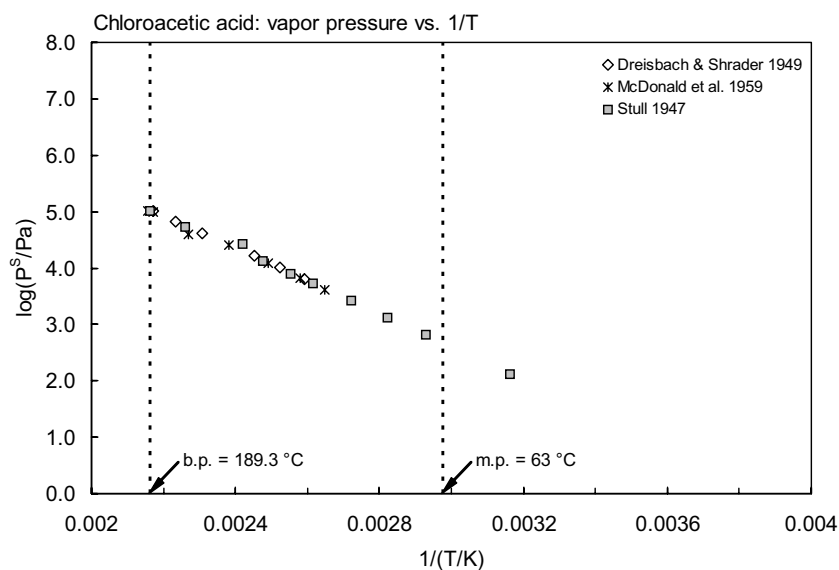
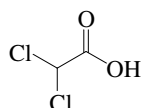


FIGURE 13.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for chloroacetic acid.

13.1.1.12 Dichloroacetic acid



Common Name: Dichloroacetic acid

Synonym: dichloroethanoic acid

Chemical Name: dichloroacetic acid

CAS Registry No: 79-43-6

Molecular Formula: $C_2H_2Cl_2O_2$, $Cl_2CHCOOH$

Molecular Weight: 128.942

Melting Point ($^{\circ}C$):

13.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

194.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5634 (Weast 1982–83)

1.5630 (Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

82.50 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

1.26 (Dean 1985)

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

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37.94* (extrapolated-regression of tabulated data, temp range 44 – $194.4^{\circ}C$, Stull 1947)

133.3 ($44^{\circ}C$, Stull 1947; quoted, Verschueren 1983)

$\log(P/mmHg) = [-0.2185 \times 12952.9/(T/K)] + 8.946605$; temp range 44 – $194.4^{\circ}C$ (Antoine eq., Weast 1972–73)

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

$\log(P_L/kPa) = 7.47122 - 2385.6/(-31.197 + T/K)$, temp range 317 – $468\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -7.2806 - 3.3706 \times 10^3/(T/K) + 9.3771 \cdot \log(T/K) - 2.0832 \times 10^{-2} \cdot (T/K) + 9.5091 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – $686\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00085 (partial pressure equilibrium, Bowden et al. 1998)

$\ln[(K_H'/(mol\ kg^{-1}\ atm^{-1}))] = -15.1776 + 8010.6/(T/K)$; temp range 5 – $35^{\circ}C$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 ($20^{\circ}C$, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.776 - 3352/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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

0.92 (recommended, Sangster 1993)

0.92 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 8.5 ppm/min per gram catalyst (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.12.1

Reported vapor pressures of dichloroacetic acid at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}C$	P/Pa
44.0	133
69.8	666.6
82.6	1333
96.3	2666
111.8	5333
121.5	7999
134.0	13332
152.3	26664
173.7	53329
194.4	101325
mp/ $^{\circ}C$	9.7

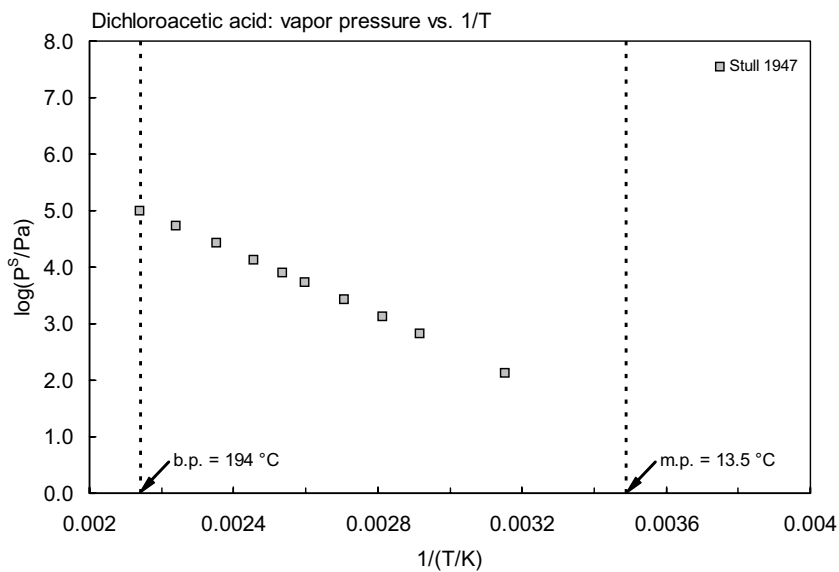
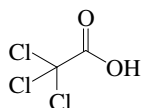


FIGURE 13.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for dichloroacetic acid.

13.1.1.13 Trichloroacetic acid



Common Name: Trichloroacetic acid

Synonym: TCA

Chemical Name: trichloroacetic acid (α or β)

CAS Registry No: 76-03-9

Molecular Formula: Cl_3CCOOH

Molecular Weight: 163.39

Melting Point ($^{\circ}\text{C}$):

59.2 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

196.5 (Lide 2003)

Density (g/cm^3 at 20°C):

1.620 (25°C , Weast 1982–83)

Molar Volume (cm^3/mol):

100.3 (61°C , Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

0.70 (Weast 1982–83)

0.52 (Dean 1985)

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

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

17.78, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.462 (mp at 59.2°C)

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

114550 (calculated- ΔS_{fus} and mp, Yalkowsky & Valvani 1980)

191860 (calculated-mp, Yalkowsky & Valvani 1980)

13000 (Verschuereen 1983)

1200000 (120 in 100 parts solvent, Dean 1985)

38300 (calculated-group contribution method, Kühne et al. 1995)

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

21.88* (extrapolated-regression of tabulated data, temp range 51 – 195.6°C , Stull 1947)

4620* (112.62°C , ebulliometry, measured range 112.62 – 197.93°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.31057 - 1618.97/(167.882 + t/^{\circ}\text{C})$; temp range 112.6 – 197.94°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log(P/\text{mmHg}) = [-0.2185 \times 13817.0/(T/\text{K})] + 9.341430$; temp range 51 – 195.6°C (Antoine eq., Weast 1972–73)

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

$\log(P/\text{kPa}) = 6.4026 - 1597.434/(165.711 + t/^{\circ}\text{C})$; temp range 112.6 – 197.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

66.14 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.2730 - 1594.3/(165.4 + t/^{\circ}\text{C})$; temp range 112 – 198°C (Antoine eq., Dean 1985, 1992)

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

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

$\log(P_L/\text{kPa}) = 6.43547 - 1618.97/(-105.268 + T/\text{K})$; temp range 326 – 473 K (Antoine eq., Stephenson & Malanowski 1987)

133.3, 491 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 63.4449 - 3.6769 \times 10^3/(T/\text{K}) - 21.13 \cdot \log(T/\text{K}) + 1.0777 \times 10^{-2} \cdot (T/\text{K}) + 4.8481 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 258 – 491 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.000137 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1}))] = -17.836 + 8660.09/(T/K)$; temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000834 (20°C , selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.931 - 3634/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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

1.33 (recommended, Sangster 1993)

1.33 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

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

Volatilization:

Photolysis: no photocatalyzed mineralization by the presence of TiO_2 as compared to both dichloroacetic acid and trichloroacetic acid (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.13.1

Reported vapor pressures of trichloroacetic acid 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)
$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)		
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)		
Stull 1947		McDonald et al. 1959		
summary of literature data		ebulliometry		
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	
51.0	133	112.62	4620	
76.0	666.6	118.13	5949	
88.2	1333	122.75	7326	
101.8	2666	129.99	9998	
116.3	5333	168.75	42302	
125.9	7999	183.92	68210	
137.8	13332	194.91	94156	
155.4	26664	196.49	98175	
175.2	53329	197.02	99584	
195.6	101325	197.48	100901	
		197.93	102318	
mp/ $^\circ\text{C}$	57.0	mp/ $^\circ\text{C}$	59.16	
		eq. 2	P/mmHg	
		A	7.31057	
		B	1618.97	
		C	167.882	

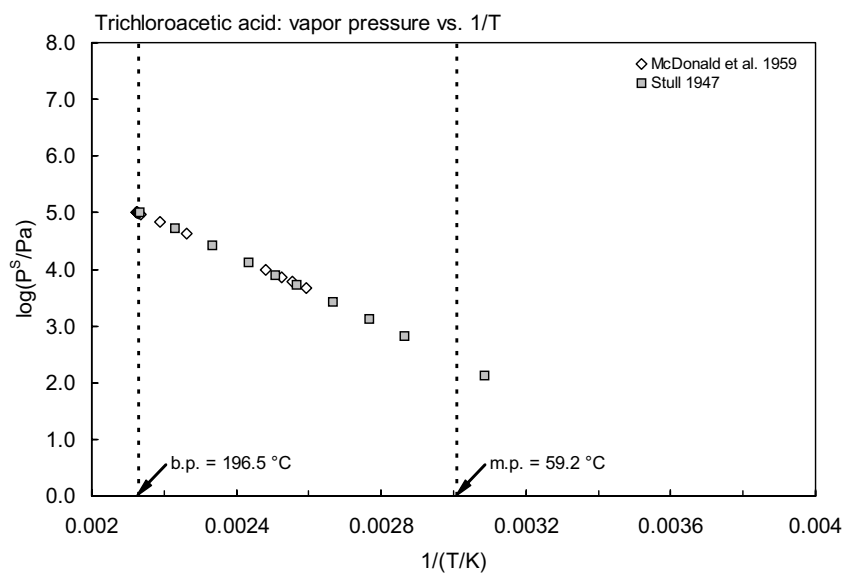
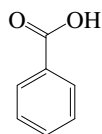


FIGURE 13.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for trichloroacetic acid.

13.1.2 AROMATIC ACIDS**13.1.2.1 Benzoic acid**

Common Name: Benzoic acid

Synonym:

Chemical Name: benzoic acid

CAS Registry No: 65-85-0

Molecular Formula: $C_7H_6O_2$, C_6H_5COOH

Molecular Weight: 122.122

Melting Point ($^{\circ}C$):

122.35 (Lide 2003)

Boiling Point ($^{\circ}C$):

249.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2659 ($15^{\circ}C$, Weast 1982–83)

1.0800 (Dean 1985)

Molar Volume (cm^3/mol):

113.6 ($130^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.20 (McDaniel & Brown 1958)

4.33 ± 0.02 , 4.38 ± 0.03 (HPLC, Unger et al. 1978)

4.08 (shake flask-TN, Clarke 1984)

4.05 ± 0.01 (equilibrium titration, Clarke & Cahoon 1987)

4.204 (Dean 1985; Lee et al. 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

69.2 (395.2 K, de Kruif & Block 1982)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

94.5 ($25^{\circ}C$, average value, Malaspina et al. 1973)

90.6 (Colomina et al. 1982)

90.51 (Ribeiro da Silva et al. 1995)

89.71 (Li et al. 2002)

90.1 (Li et al. 2004)

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

18.0 (Tsonopoulos & Prausnitz 1971)

18.2 (395.2 K, de Kruif & Block 1982)

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

45.61 (Tsonopoulos & Prausnitz 1971)

43.81 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.111 (mp at $122.35^{\circ}C$)

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

3340* ($24.6^{\circ}C$, shake flask-synthetic method, Ward & Cooper 1930)

3298* (shake flask-thermostatic and synthetic methods, measured range 25 – $88.6^{\circ}C$, Morrision 1944)

4200 (shake flask-liquid scintillation counting, Lu & Metcalf 1975)

3600 (shake flask-UV, Yalkowsky et al. 1983)

3416* (shake flask-weight titration, measured temp range 5 – $65^{\circ}C$, Strong et al. 1989)

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

- 799.9* (122.2°C, static method-manometer, measured range 122.2–249.0°C, Kahlbaum 1898)
 6.893* (60.1°C, isoteniscope method, measured range 60.1–247°C, Klosky et al. 1927)
 $\log(P_s/\text{mmHg}) = 11.956 - 4409/(T/K)$; temp range 61–121°C (solid, isoteniscope, Klosky et al. 1927)
 $\log(P_L/\text{mmHg}) = 30.172 - 4714/(T/K) - 6.720 \cdot \log(T/K)$; temp range 128–247°C (liquid, isoteniscope, Klosky et al. 1927)
 0.840* (extrapolated-regression of tabulated data, temp range 96–227°C, Stull 1947)
 12.35* (70.48°C, transpiration method, measured range 70.48–114.11°C, Davies & Jones 1954)
 $\log(P/\text{mmHg}) = 12.8699 - 4775.7/(T/K)$, temp range 70.48–114.11°C (transpiration, Davies & Jones 1954)
 0.160* (298.3 K, Knudsen effusion, measured range 290.4–315.5 K, Wiedemann 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 15253.3/(T/K)] + 9.03300$; temp range 60–110°C (Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 16295.1/(T/K)] + 9.741362$; temp range 96–249.2°C (Antoine eq., Weast 1972–73)
 0.160* (Knudsen effusion weight-loss method, fitted to Antoine eq., measured range 65.05–110.25°C, Malaspina et al. 1973)
 $\log(P/\text{mmHg}) = (12.175 \pm 0.040) - (4501 \pm 17)/(T/K)$; temp range 338–383 K (Antoine eq., Knudsen effusion, Malaspina et al. 1973)
 0.108* (effusion method, measured range 25–70.5°C, DePablo 1976)
 16.8* (71.25°C, isoteniscope method, measured range 344.4–393.8 K, Sachinidis & Hill 1980)
 $\log(P/\text{mmHg}) = 12.45 - 4605/(T/K)$; temp range 344.4–393.8 K (isoteniscope method, Sachinidis & Hill 1980)
 0.070*, 0.050* (20°C, gas saturation method, vapor pressure balance, OECD 1981)
 0.112* (25.25°C, Knudsen effusion method, temp range 20.25–40.25°C, Colomina et al. 1982)
 $\log(P/\text{Pa}) = (14.87 \pm 0.02) - (4719.6 \pm 7.1)/(T/K)$; temp range 293.4–313.4 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)
 0.0907 (20°C, evaporation method, Gückel et al. 1982)
 0.105* (diaphragm manometer/torsion mass-loss effusion, extrapolated from measured range 316–391 K, de Kruif & Block 1982)
 0.109 ± 0.005 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
 0.9505 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 9.033 - 3333.3/(T/K)$, temp range 60–110°C (Antoine eq., Dean 1985, 1992)
 0.105 (solid P_s , interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 15.94025 - 7420.596/(74.333 + T/K)$; temp range 294–321 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 11.8285 - 4719.5/(T/K)$; temp range 343–373 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
 0.772 (liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.80911 - 2776.12/(-43.978 + T/K)$; temp range 405–523 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 0.600 (20°C, OECD 1981; quoted, Howard 1989)
 $\log(P/\text{mmHg}) = -140.0388 + 80.479/(T/K) + 62.611 \cdot \log(T/K) - 6.5321 \times 10^{-2} \cdot (T/K) + 2.4596 \times 10^{-5} \cdot (T/K)^2$; temp range 396–751 K (vapor pressure eq., Yaws 1994)
 0.13* (26°C, Knudsen effusion, measured range 26–50°C, Li et al. 2002)
 $\ln(P/\text{Pa}) = (34.031 \pm 0.30) - (10790 \pm 93)/(T/K)$; temp range 299–323 K (Knudsen effusion technique, Li et al. 2002)
 $\ln(P/\text{Pa}) = 34.320 - 10866/(T/K)$; temp range 304–317 K (regression eq. of Ribeiro da Silva et al. 1995 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (34.181 \pm 0.446) - (10836 \pm 140)/(T/K)$; temp range 299–328 K (Knudsen effusion technique, Li et al. 2004)

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

- 0.00709 (Howard 1989)
 0.00575; 0.0110 (calculated-P/C, calculated-bond contribution, Meylan & Howard 1991)
 0.00415 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

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

- 1.87 (shake flask-UV, Fujita et al. 1964)
- 1.68 (shake flask-UV, Halmekoski & Hannikainen 1964)
- 1.85 \pm 0.01 (shake flask-UV, Iwasa et al. 1965)
- 2.03 (shake flask-LSC, Lu & Metcalf 1975)
- 1.78 \pm 0.01, 1.77 \pm 0.01 (HPLC- k' correlation, Unger et al. 1978)
- 1.79 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
- 1.86, 1.87 (calculated-fragment const., Rekker 1977)
- 1.94 (RP-HPLC correlation, Hanai & Hubert 1982)
- 1.95 (HPLC- k' correlation; Miyake & Terada 1982)
- 1.87 (microelectrometric titration, Clarke 1984)
- 2.18 \pm 0.03; 2.03 (exptl.-ALPM, selected best lit. value, Garst & Wilson 1984)
- 1.44, 1.87 (HPLC- k' correlation, Haky & Young 1984)
- 1.88 (shake flask-UV at pH 0.5, Nishimura et al. 1985)
- 1.97 (microelectrometric titration, Clarke & Cahoon 1987)
- 1.94 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.93 (HPLC- k' correlation, Miyake et al. 1987)
- 1.88 (CPC, Berthod et al. 1988)
- 1.85 \pm 0.04 ("Filter Chamber"-UV, Hersey et al. 1989)
- 1.87 (recommended, Sangster 1989, 1993)
- 1.88 (back flashing-CPC centrifugal partition chromatography, Menges et al. 1990)
- 1.87 (recommended, Hansch et al. 1995)

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

- 1.32, 2.00, 2.14 (fish, algae, mosquito, Lu & Metcalf 1975)
- 3.26, 3.45 (daphnia, snail, Lu & Metcalf 1975)
- 0.48 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
- 1.43 (alga *Chlorella fusca*, calculated- K_{ow} , Geyer et al. 1984)
- < 1.0 (golden ide, Freitag et al. 1985)
- < 1.0 (algae, Freitag et al. 1985)
- 3.11 (activated sludge, Freitag et al. 1985)
- 1.15 (trout muscle, calculated- K_{ow} , Branson 1978)

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

- 1.26; 1.86; 0.602 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 1.50 (soil, quoted exptl., Meylan et al. 1992)
- 1.16 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization: rate of evaporation $k = 1.89 \times 10^{-8} \text{ mol cm}^{-2} \text{ h}^{-1}$ at 20°C determined by evaporation method (Gückel et al. 1982).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.0 \text{ d}$, based on estimated vapor-phase reaction with hydroxyl radical in air (Howard 1989).

Hydrolysis: $k = 4.3 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for reactions of hydroxyl radical in aqueous solution (Buxton et al. 1986)

$k = 1.15 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ (Mabury & Crosby 1996);

$k(\text{exptl}) = 1.2 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ for reaction with hydroxy radical (Armbrust 2000)

Biodegradation: completely degraded by a soil microflora after 24 h (Alexander & Lustigman 1966; quoted, Verschueren 1983);

completely degraded for 16 mg/L concn. within one day by soil and by wastewater (Haller 1978);

$t_{1/2} \sim 0.2\text{--}3.6$ d if released into water, should readily biodegrade (Howard 1989);
average $k(\text{exptl}) = 0.11533 \text{ h}^{-1}$ compared to group method predicted $k = 0.0993 \text{ h}^{-1}$ (nonlinear) and $k = 0.0263 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation: degradation $k = 6.84 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.0$ d for reactions with photochemically produced hydroxyl radical (Howard 1989).
Surface water: if released into water, should readily biodegrade with an estimated $t_{1/2} = 0.2\text{--}3.6$ d (Howard 1989).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 13.1.2.1.1
Reported aqueous solubilities of benzoic acid at various temperatures

Ward & Cooper 1930		Morrison 1944		Strong et al. 1989	
shake flask-synthetic method		thermostatic and synthetic		shake flask-weight titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
24.6	3340	25.0	3298	5	1830
42.4	6280	35.0	4641	15	2482
57.8	10930	45.0	6167	25	3416
74.1	20670	55.4	10137	35	4776
83.1	31300	60.2	12213	45	6656
88.3	39660	64.6	14533	55	9629
		68.5	16976	65	14325
		75.1	22838		
		79.3	26991		
		82.1	31021		
		88.6	43356		

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 23.29$
25°C

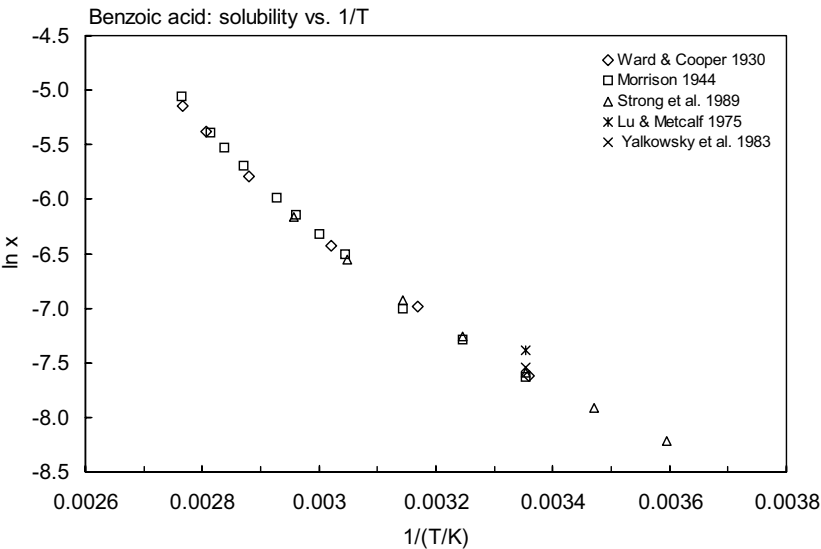


FIGURE 13.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzoic acid.

TABLE 13.1.2.1.2

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

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{aligned}$$

1.

Kahlbaum 1898		Klosky et al. 1927		Stull 1947		Davies & Jones 1954	
static method-manometer*		isoteniscope method		summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid							
122.2	799.9	60.1	6.893	96.0	133.3	70.48	12.35
132.5	1333	80.4	41.06	119.5	666.6	75.14	19.33
146.5	2666	100.2	190.1	132.1	1333	80.43	31.02
155.5	4000	121.0	777.3	146.7	2666	84.47	44.0
161.9	5333			162.6	5333	89.88	68.66
167.2	6666	eq. 1	P/mmHg	172.8	7999	95.35	108.9
178.5	9999	A	11.956	186.2	13332	100.59	149.2
185.9	13332	B	4409	205.8	26664	105.05	230.8
196.5	19998			227.0	53329	109.85	341.0
204.9	26664		liquid	249.2	101325	114.11	458.1
211.5	33331	128.6	1120				
217.0	39997	134.5	1573	mp/°C	121.7	eq. 1	P/mmHg
225.8	53329	148.0	2960			A	12.8699
233.8	66661	158.2	4533			B	4775.7
239.8	79993	172.8	8506				
245.5	93326	187.6	14772			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 91.42$	
249.0	101325	199.7	22238			at 365.5 K	
		216.2	38224			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.37$	
		233.0	63835			at 298.15 K	
		247.0	95739				
		eq. 4	P/mmHg				
		A	30.172				
		B	4714				
		C	6.720				

*complete list see [ref.](#)

2.

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
gas saturation							
290.4	0.0613	65.05	9.879	344.4	16.80	10	0.02
294.4	0.118	71.35	16.72	352.8	37.73	20	0.07
298.3	0.160	74.65	23.91	373.7	167.6	30	0.24
299.8	0.205	77.95	29.69	393.8	733.5	40	0.76
300.5	0.244	85.25	55.02			50	2.20
301.1	0.220	89.15	76.1	eq. 1	P/mmHg	vapor pressure balance	
304.4	0.337	94.05	112.5	A	12.45	10	0.012
315.5	1.173	99.75	169.2	B	4605	20	0.05

TABLE 13.1.2.1.2 (Continued)

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
293.36	0.0889*	105.05	255.3	$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 88.1$		30	0.17
293.56	0.0907*	110.25	362.7			40	0.56
293.36	0.0893*					50	1.70
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.92$					
		at 298.15 K					
eq. 1	P/mmHg			DePablo 1976			
A	12.2937		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.18$	effusion method			
B	4530.02		at 360.8 K	t/°C	P/Pa		
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 86.61$		eq. 1	P/mmHg				
		A	12.175	25	0.108		
*different orifice areas of		B	4501	45	1.03		
Knudsen effusion cell		temp range 338.2–383.4 K		70.25	11.92		
		calculated average value					
		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.5$					
		at 298 K					

3.

Colomina et al. 1982		de Kruif & Block 1982		Li et al. 2002	
Knudsen effusion		manometer/effusion		Knudsen effusion	
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
293.4	0.0604	316.4	0.89	299.15	0.13
293.67	0.063	321.01	1.44	303.25	0.22
295.5	0.0781	321.25	1.48	308.15	0.38
295.75	0.0814	323.58	1.9	313.15	0.66
296.59	0.09	328.73	3.25	318.15	1.13
298.38	0.112	329.01	3.34	323.15	1.86
298.95	0.119	335.67	6.44		
301.19	0.157	338.66	8.6	eq. 1a	P/Pa
301.71	0.167	344.64	14.74	A	34.031
304.47	0.23	347.6	19.6	B	10790
305.15	0.25	350.01	24.17		
307.6	0.334	353.14	31.79		
308.11	0.354	359.05	52.37		
308.34	0.365	361.41	63.5		
310.14	0.445	364.96	84.69		
311.17	0.503	367.77	106.4		
311.29	0.508	368.43	111.9		
313.38	0.64	383.04	334.8		
		390.93	588.4		
eq. 1	P/Pa				
A	14.87	Data fitted to 3-parameter			
B	4719.6	vapor-pressure eq. see ref.			
		at 395.52K			
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 90.6 \pm 0.2$		$\Delta H_{\text{v}}/(\text{kJ/mol}) = 69.2$			
temp range 293–313 K		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 87.4$			
		$\Delta H_{\text{fus}}/(\text{kJ/mol}) = 18.0$			

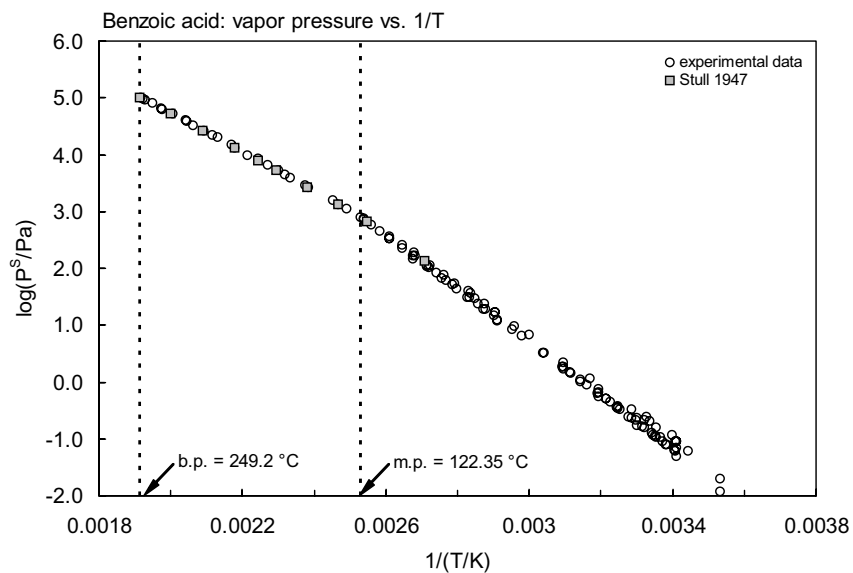
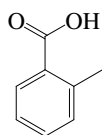


FIGURE 13.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzoic acid.

13.1.2.2 2-Methyl benzoic acid (*o*-Toluic acid)

Common Name: *o*-Toluic acid

Synonym: 2-methyl benzoic acid

Chemical Name: *o*-toluic acid, 2-methyl benzoic acid

CAS Registry No: 118-90-1

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

103.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

259 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.062 (115 $^{\circ}C$, Weast 1982–83; Verschueren 1983)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

3.91 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.91 (Weast 1982–83)

3.90 (Dean 1985)

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

20.17 (Tsonopoulos & Prausnitz 1971)

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

53.56 (Tsonopoulos & Prausnitz 1971)

53.5, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.170 (mp at $103.5^{\circ}C$)

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

22300* (85.1 $^{\circ}C$, shake flask-residue volume, measured range 85.1–102.4 $^{\circ}C$, Sidgwick et al. 1915)

1185 (shake flask, Fühner 1924)

1162* (shake flask-weight titration, measured range 5–65 $^{\circ}C$, Strong et al. 1989)

1074* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P/mmHg) = -35.8816 - 3.2354 \times 10^3/(T/K) + 21.133 \cdot \log (T/K) - 3.0165 \times 10^{-2} \cdot (T/K) + 1.1587 \times 10^{-5} \cdot (T/K)^2$;
temp range 377–751 K (vapor pressure eq., Yaws 1994)

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

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

2.18 (shake flask-UV, Tomida et al. 1978)

2.81 (Scherrer & Howard 1979)

2.46 (shake flask at pH 1, Hansch & Leo 1987)

2.27 (shake flask-UV at pH 2, Da et al. 1992)

2.46 (recommended, Sangster 1993)

2.46 (recommended, pH 1, Hansch et al. 1995)

1.72 (RP-HPLC-RT correlation on short ODP column, pH 2, Donovan & Pescatore 2002)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.2.1

Reported aqueous solubilities of 2-methylbenzoic acid (*o*-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
85.1	22300	5	568.3	20	825
109.1	36600	15	806.6	25	1074
118.3	50000	25	1162	35	1620
130.4	69900	35	1695	40	1883
143.7	102000	45	2522		
156.5	202300	55	3778		
160.2	314700	65	5775		
161.2	399200				
160.2	486300	$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 28.92$			
154.6	601600	25°C			
147.4	701200				
119.8	846400				
97.2	905300				
93.7	918800				
94.4	938300				
96.0	959500				
102.4	1000000				
critical solution temp 161.2°C					
triple point 93.5°C					
mp 102.4°C					

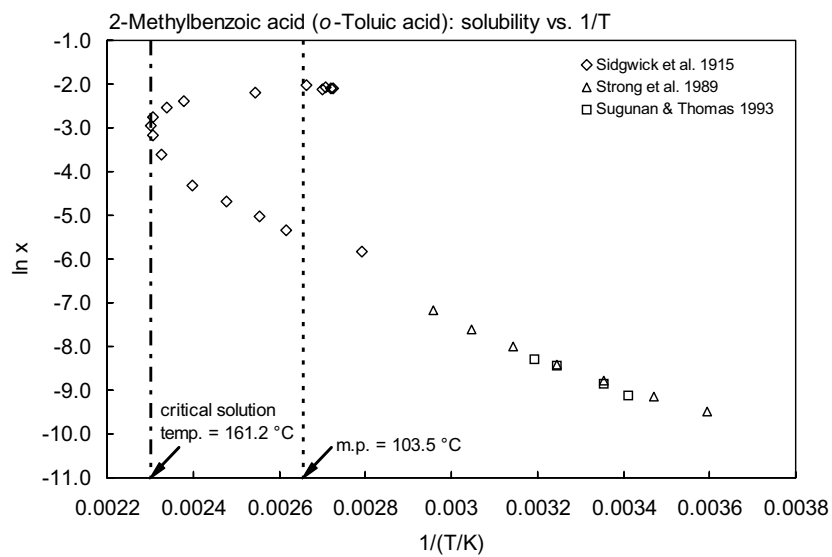
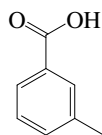


FIGURE 13.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylbenzoic acid.

13.1.2.3 3-Methyl benzoic acid (*m*-Toluic acid)

Common Name: *m*-Toluic acid

Synonym: 3-methyl benzoic acid

Chemical Name: *m*-toluic acid, 3-methyl benzoic acid

CAS Registry No: 99-04-7

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

109.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

263.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

1.054 ($112^{\circ}C$, Weast 1982–83; Verschuereen 1983)

Molar Volume (cm^3/mol):

129.2 ($112^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.270 (Weast 1982–83)

4.269 (Dean 1985)

4.220 (Sangster 1993)

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

15.73 (Tsonopoulos & Prausnitz 1971)

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

10.96 (Tsonopoulos & Prausnitz 1971)

41.17, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.147 (mp at $109.9^{\circ}C$)

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

11600* ($80^{\circ}C$, shake flask-residue volume, measured range 80 – $110.5^{\circ}C$, Sidgwick et al. 1915)

982 (shake flask-residue volume method, Fühner 1924)

1700 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

872* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

1246* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P_L/kPa) = 8.1472 - 3280.8/(T/K)$, temp range 473 – $533 K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

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

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

2.37 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.43 (HPLC- k' correlation, Miyake & Terada 1982)

2.41 (shake flask-AS, Miyake et al. 1987)

2.39 (centrifugal partition chromatography CPC, Terada et al. 1987)

2.44; 2.47 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.38 (shake flask-UV at pH 2, Da et al. 1992)

- 2.37 (recommended, Sangster 1993)
 2.37 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

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

Half-Lives in the Environment:

TABLE 13.1.2.3.1

Reported aqueous solubilities of 3-methylbenzoic acid (*m*-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
80	11600	5	449.3	20	1070
89.8	15300	15	621	25	1246
118.6	31300	25	872	35	1544
140.5	58800	35	1270	40	1720
153.3	99600	45	1852		
162.2	299400	55	2754		
162.1	401100	65	4115		
160.7	501000	75	6492		
157.7	601500				
145.1	711700	$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 26.15$			
129.6	795700				
121.8	820600				
105.9	866700				
96.4	893200				
94.2	924500				
101.9	969300				
110.5	1000000				
critical solution temp 162.2°C					
triple point		142.0°C			
mp		110.5°C			

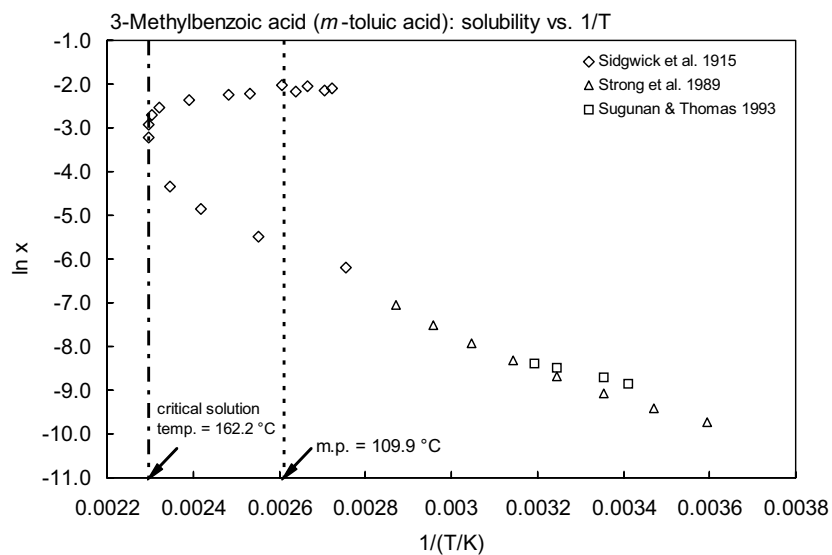
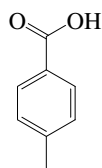


FIGURE 13.1.2.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-methylbenzoic acid (*m*-toluic acid).

13.1.2.4 4-Methyl benzoic acid (*p*-Toluic acid)

Common Name: *p*-Toluic acid

Synonym: 4-methyl benzoic acid

Chemical Name: *p*-toluic acid, 4-methyl benzoic acid

CAS Registry No: 99-94-5

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

179.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

275.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

4.37, 4.30 ± 0.09 (quoted, HPLC, Unger et al. 1978)

4.37, 4.41 ± 0.01 (quoted, HPLC, Unger et al. 1978)

4.36 (Weast 1982–83)

4.37, 4.26 (quoted, shake flask-TN, Clarke 1984)

4.362 (Dean 1985)

4.39 (Sangster 1993)

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

22.72 (Tsonopoulos & Prausnitz 1971)

23.81 (differential scanning calorimetry, Li et al. 2001)

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

50.21 (Tsonopoulos & Prausnitz 1971)

50.21, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.0304 (mp at $179.6^{\circ}C$)

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

11600* (100, shake flask-residue volume, measured range 100 – $176.8^{\circ}C$, Sidgwick et al. 1915)

383 (selected, Tsonopoulos & Prausnitz 1971)

343* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

331* (shake flask-UV, Sugunan & Thomas 1993)

378.5* (shake flask-titration, measured range 278.15 – $343.15\ K$, Apelblat & Manzurola 1999)

$\ln [m/(mol\ kg^{-1})] = -264.605 - 9059.53/(T/K) + 40.069 \cdot \ln (T/K)$; temp range 278 – $343\ K$ (shake flask-titration, Apelblat & Manzurola 1999)

371* (shake flask-laser monitoring observation technique, measured range 288.35 – $370.95\ K$, Li et al. 2001)

393* ($26.4^{\circ}C$, synthetic method-laser technique, measured range 290.25 – $348.45\ K$, Chen & Ma 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

30.93* ($95.20^{\circ}C$, Knudsen effusion, measured range 95.2 – $134.96^{\circ}C$ (Davies & Jones 1954)

$\log (P/mmHg) = 128585 - 4968.7/(T/K)$; temp range 95.2 – $134.96^{\circ}C$ (Knudsen effusion, Davies & Jones 1954)

$\log (P/mmHg) = -67.6587 - 2.2339 \times 10^3/(T/K) + 33.347 \cdot \log (T/K) - 3.7709 \times 10^{-2} \cdot (T/K) + 1.313 \times 10^{-5} \cdot (T/K)^2$; temp range 453 – $773\ K$ (vapor pressure eq., Yaws 1994)

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

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

- 2.27 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)
- 2.22 \pm 0.02, 2.26 \pm 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.36 (shake flask-UV at pH 2, Ezumi & Kubota 1980)
- 2.43 (calculated-HPLC- k' correlation, Miyake & Terada 1982)
- 2.34 (electrometric titration, Clarke 1984)
- 2.67 (HPLC-RT correlation, Garst 1984)
- 2.66 (centrifugal partition chromatography CPC, Terada et al. 1987)
- 2.38; 2.41 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
- 2.35 (HPLC-RT correlation, Jenke et al. 1990)
- 2.26 (shake flask-UV at pH 2, Da et al. 1992)
- 2.34 (recommended, Sangster 1994)
- 2.27 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

- 2.15, 1.15, 1.30 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.77 (soil, quoted exptl., Meylan et al. 1992)
- 1.37 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

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

Biotransformation:

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

Half-Lives in the Environment:

TABLE 13.1.2.4.1

Reported aqueous solubilities of 4-methylbenzoic acid (*p*-toluic) acid at various temperatures

1.

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
100	11600	5	177.8	20	263	5.0	201.5
110	13600	15	243.5	25	331	11.0	249.2
114.4	15100	25	343	35	466	17.0	271.0
133.7	29600	35	486	40	534	21.5	309.1
141.4	49700	45	695			25.0	378.5
150.9	100800	55	1008			25.5	318.6
157.9	202700	65	1485			30.0	469.8
159.1	301400					30.0	488.8
158.5	405700	$\Delta H_{sol}/(kJ\ mol^{-1}) = 26.74$ 25°C				35.0	499.7
158.0	503800					35.0	501.1
152.6	605500					35.0	502.4
145.1	796800					40.0	593.7

TABLE 13.1.2.4.1 (Continued)

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
156.5	925200					40.0	595.0
176.8	1000000					40.0	638.6
						45.0	721.7
Critical solution temp	159.1°C					50.0	887.8
Triple point	142°C					52.0	912.3
mp	176.8°C					55.0	1062
						58.0	1185
						60.0	1283
						61.0	1389
						65.0	1525
						67.0	1702
						70.0	1865
							$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$
							at 298.15 K
							$\ln S = A + B/T + C \ln T$
							S mol·kg ⁻¹
							A -264.605
							B 9059.53
							C 40.069

2.

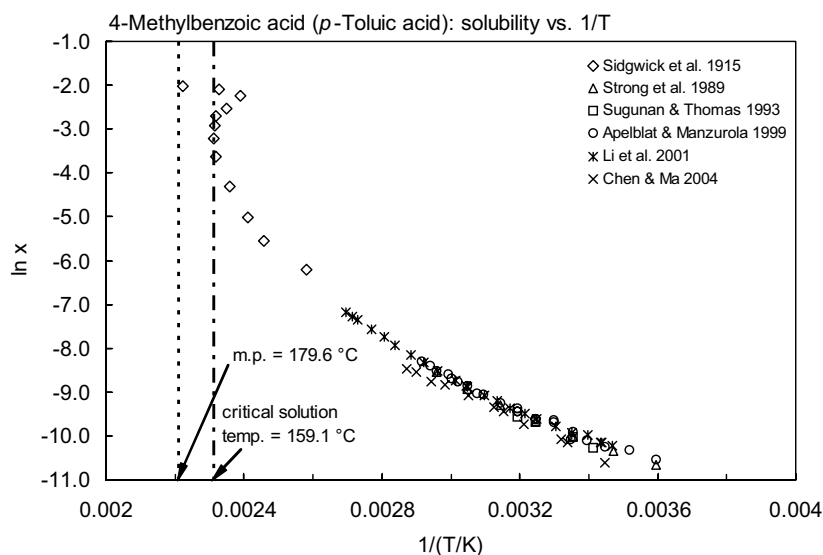
Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
15.2	272.3	290.25	185.0
17.8	295	299.55	292.7
17.9	295	301.25	315.3
21.3	347.6	311.25	448.6
25.2	370.7	317.25	596.4
29.4	423.6	320.05	657.0
34.7	506.8	327.75	857.8
37.8	567.3	335.35	1109
42.1	650.5	339.85	1190
46.0	756.4	344.95	1465
49.8	869.9	348.35	1570
55.1	1051		
55.3	1074		
58.6	1210		
64.4	1520		
69.1	1838		
73.7	2201		
79.1	2723		
83.3	3260		
87.7	3911		

(Continued)

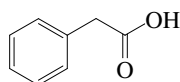
TABLE 13.1.2.4.1 (Continued)

Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
93.1	4834		
95.5	5204		
97.8	5726		

$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.81$

FIGURE 13.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-methylbenzoic acid (*p*-toluic acid).

13.1.2.5 Phenylacetic acid



Common Name: Phenylacetic acid

Synonym: phenylethanoic acid, α -toluic acid, benzenecetic acid

Chemical Name: phenylacetic acid

CAS Registry No: 103-82-2

Molecular Formula: $C_8H_8O_2$, $C_6H_5CH_2COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

76.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

265.5 (Stull 1947; Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.081 (Verschuereen 1983)

Molar Volume (cm^3/mol):

124.8 ($77^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.28 ($18^{\circ}C$, Weast 1982–83)

4.31 (Sangster 1989)

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

17.11 (Tsonopoulos & Prausnitz 1971)

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

48.95 (Tsonopoulos & Prausnitz 1971)

41.42, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.312 (mp at $76.5^{\circ}C$)

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

17700* (thermostatic and synthetic methods, measured range 25 – $86.7^{\circ}C$, Morrison 1944)

16600 ($20^{\circ}C$, Hodgman 1952)

17790 (selected, Tsonopoulos & Prausnitz 1971)

16600 ($20^{\circ}C$, quoted, Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.835 (extrapolated-regression of tabulated data, temp range 97 – $265^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 15568.7/(T/K)] + 9.206178$; temp range 97 – $265.5^{\circ}C$ (Antoine eq., Weast 1972–73)

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

$\log(P/kPa) = 8.00148 - 3144.95/(-14.408 + T/K)$; temp range 370 – $539 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0056 (calculated-P/C)

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

1.41 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971)

1.41 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.51 (shake flask-UV, Yaguzhinskii et al. 1973)

1.94 (RP-LC-RT correlation, Hanai & Hubert 1982)

1.45 (shake flask-UV at pH 3.5, Kuchar et al. 1982)

1.95 ± 0.04 ; 1.51 (exptl.-ALPM, selected best lit. value, Garst 1984)

1.41 (recommended, Sangster 1989, 1993)

1.34 ± 0.14, 1.07 ± 0.49 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k' correlation, Cichna et al. 1995)

1.41 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

1.49, 1.42, 1.45 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

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

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

1.45 (soil, quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.5.1

Reported aqueous solubilities of phenylacetic acid at various temperatures:

Morrison 1944

thermostatic and synthetic

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
25.0	17700
35.0	26005
45.0	39484
41.5	39211
58.4	49695
68.8	59225
76.5	69845
83.0	83188
86.7	93399

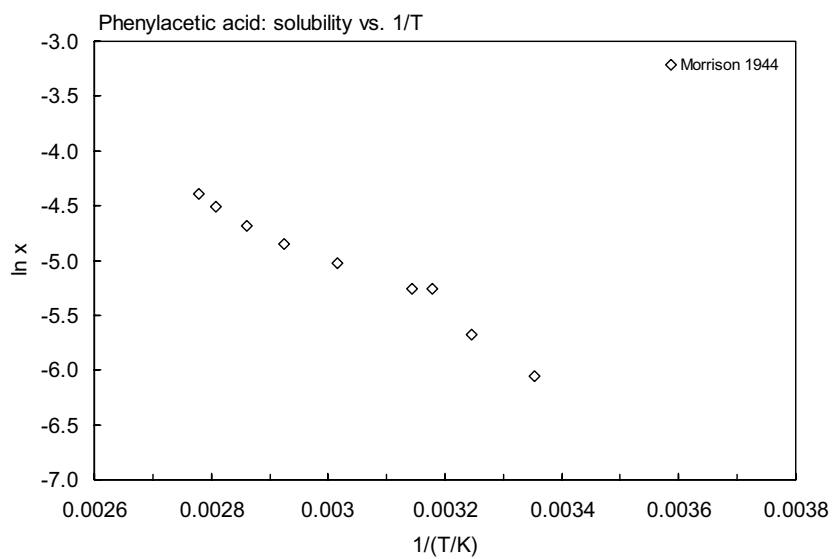
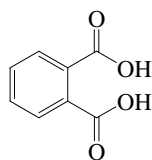


FIGURE 13.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phenylacetic acid.

13.1.2.6 Phthalic acid



Common Name: Phthalic acid

Synonym: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

Chemical Name: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

CAS Registry No: 88-99-3

Molecular Formula: $C_8H_6O_4$, $C_6H_4-1,2-(COOH)_2$

Molecular Weight: 166.132

Melting Point ($^{\circ}C$):

230 (dec., Lide 2003)

Boiling Point ($^{\circ}C$):

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.593 (Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

2.89, 5.51 (pK_1 , pK_2 , Weast 1982–83)

2.95, 5.408 (pK_1 , pK_2 , Dean 1985)

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

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

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

7014* (shake flask-synthetic method, measured range 25 – $85^{\circ}C$, McMaster et al. 1921):

7160* ($25.8^{\circ}C$, shake flask-synthetic method, measured range 25.8 – $113.8^{\circ}C$, Ward & Cooper 1930)

5400 ($14^{\circ}C$, Verschueren 1983)

6300 (Dean 1985)

7024* (shake flask, measured range 283.65 – 338.15 K, Apelblat & Manzurolo 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P/mmHg) = -90.3221 - 3.2214 \times 10^3/(T/K) + 44.109 \cdot \log(T/K) - 5.0056 \times 10^{-2} \cdot (T/K) + 1.6895 \times 10^{-5} \cdot (T/K)^2$;
temp range 464 – 800 K (vapor pressure eq., Yaws 1994)

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

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

0.79 (shake flask-UV, Tomida et al. 1978)

0.15 (electrometric titration, Freese et al. 1979)

0.73 (shake flask at pH 1, Log P Database, Hansch & Leo 1987)

0.71 ($30^{\circ}C$, shake flask-UV at pH 1, Patrunkey & Pflegel 1992)

0.73 (recommended, Sangster 1993)

0.73 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, log K_{OC} :

0.301, 1.49, 0.301	(sediment, Podzol soil, Alfidol soil, von Oepen et al. 1991)
1.07	(soil, quoted exptl., Meylan et al. 1992)
1.87	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.07	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $78.4 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 2 \text{ d}$ in initial phase, $t_{1/2} = 15 \text{ d}$ in late phase in sludge -amended soil (Roslev et al. 1998)

Biota:

TABLE 13.1.2.6.1**Reported aqueous solubilities of *o*-phthalic acid at various temperatures**

McMaster et al. 1921		Ward & Cooper 1930		Apelblat & Manzurola 1989	
shake flask-synthetic method		shake flask-synthetic method		shake flask-titration	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	T/K	$\text{S/g}\cdot\text{m}^{-3}$
25	7014	25.8	7160	283.65	2617
35	10125	43.7	13210	296.15	6546
45	14460	48.9	16470	298.15	7026
55	21680	58.0	22760	302.65	8633
65	32460	63.7	28970	307.15	9839
75	49260	77.8	53220	309.15	11020
85	78870	85.7	75940	311.15	11638
		94.8	118500	315.15	13936
		101.1	157900	317.15	15146
		113.8	294600	318.15	15164
				319.15	16705
				323.15	18893
				323.15	20554
				327.15	22926
				334.15	29783
				338.15	36955
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 29.0$					

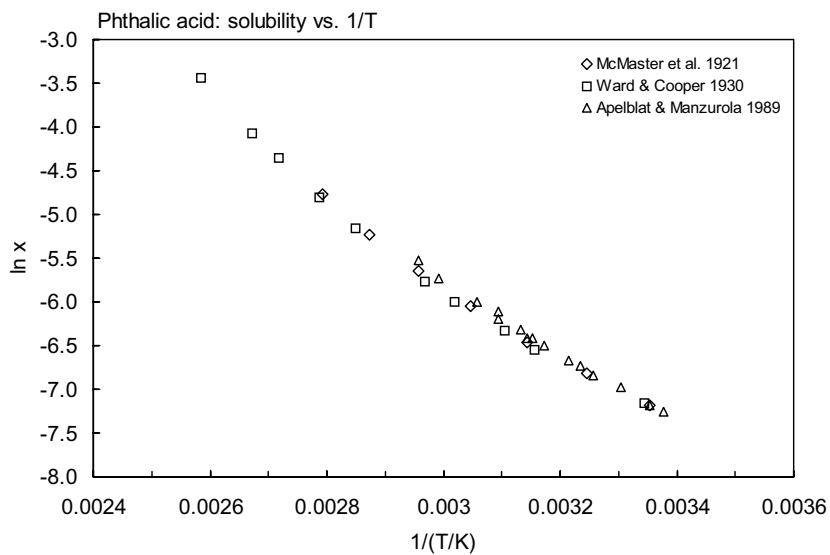
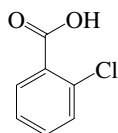


FIGURE 13.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phthalic acid.

13.1.2.7 2-Chlorobenzoic acid



Common Name: 2-Chlorobenzoic acid

Synonym: *o*-chlorobenzoic acid

Chemical Name: 2-chlorobenzoic acid, *o*-chlorobenzoic acid

CAS Registry No: 118-91-2

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

140.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschuereen 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5440 (Weast 1982–83, Verschuereen 1983)

1.5440 ($25^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

101.4 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

2.920 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968; Weast 1982–83)

2.877 (Dean 1985)

3.850 (Sangster 1993)

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

25.73 (Tsonopoulos & Prausnitz 1971)

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

62.34 (Tsonopoulos & Prausnitz 1971)

62.26, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0741 (mp at $140.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2130 (Osol & Kilpatrick 1933)

2114 (selected, Tsonopoulos & Prausnitz 1971)

2100 (Verschuereen 1983)

1100 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

$\log (P/mmHg) = -42.9847 - 3.1867 \times 10^3/(T/K) + 23.694 \cdot \log (T/K) - 3.0284 \times 10^{-2} \cdot (T/K) + 1.0828 \times 10^{-5} \cdot (T/K)^2$;
temp range 415–792 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

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

1.98 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979, 1987)

2.63; 2.56 (calculated-fragment const., calculated- π const. Rekker 1977)

2.66 (shake flask-UV, Tomida et al. 1978)

1.99 (centrifugal partition chromatography, Berthod et al. 1988)

2.02 (shake flask-UV at pH 2, Da et al. 1992)

1.99 (recommended, Sangster 1993)

2.05 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by soil microflora: $t_{1/2} > 64$ d, biodegradation by waste water at pH 7.3 and 30°C, $t_{1/2} > 25$ d, and degradation by soil suspension at pH 7.3 and 30°C; $t_{1/2} = 7\text{--}14$ d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
complete degradation of 16 mg/L by soil in 7–14 d (Haller 1978).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

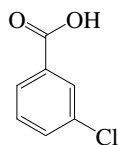
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.8 3-Chlorobenzoic acid



Common Name: 3-Chlorobenzoic acid

Synonym: *m*-chlorobenzoic acid

Chemical Name: 3-chlorobenzoic acid, *m*-chlorobenzoic acid

CAS Registry No: 535-80-8

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

158 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4960 ($25^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

104.7 ($25^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

3.82 (Weast 1982–83)

3.83 (Dean 1985)

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

23.85 (Tsonopoulos & Prausnitz 1971)

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

55.65 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.0496$ (mp at $158^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

385 (Osol & Kilpatrick 1933)

398 (selected, Tsonopoulos & Prausnitz 1971)

400 ($0^{\circ}C$, Verschueren 1983)

400 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

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

2.68 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979)

2.65, 2.52 (calculated-fragment const., calculated- π const, Rekker 1977)

0.89 (HPLC-RT correlation, Veith et al. 1979)

2.57 (HPLC- k' correlation, Miyake & Terada 1982)

2.62 (centrifugal partition chromatography, Terada et al. 1987)

2.51; 2.58 (shake flask at pH 1; HPLC-RT correlation, Wang et al. 1989)

2.72 (shake flask-UV at pH 2, Da et al. 1992)

2.60 (recommended, Sangster 1993)

2.68 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis: direct aqueous photolysis $k = 0.013 \pm 0.001 \text{ min}^{-1}$ with $t_{1/2} = 55 \text{ min}$ (Stegeman et al. 1993).

Oxidation:

Hydrolysis:

Biodegradation: decomposed by soil microflora, $t_{1/2} = 32 \text{ d}$ (Alexander & Lustigman 1966; quoted, Verschueren 1983);

complete degradation of 16 mg/L by soil and by wastewater in 7–14 d (Haller 1978).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

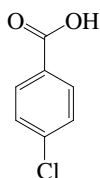
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.9 4-Chlorobenzoic acid



Common Name: 4-Chlorobenzoic acid

Synonym: *p*-chlorobenzoic acid

Chemical Name: 4-chlorobenzoic acid, *p*-chlorobenzoic acid

CAS Registry No: 74-11-3

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

243.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschueren 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.541 ($24^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

3.98 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.98 (Weast 1982–83)

3.98, 3.85 (quoted, shake flask-TN, Clarke 1984)

3.986 (Dean 1985)

3.850 (Sangster 1993)

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

32.26 (Tsonopoulos & Prausnitz 1971)

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

62.76 (Tsonopoulos & Prausnitz 1971)

62.9, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.00726$ (mp at $243^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

68.0 (Osol & Kilpatrick 1933)

72.6 (selected, Tsonopoulos & Prausnitz 1971)

77.0 (Verschueren 1983)

200 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

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

2.65 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.65; 2.52 (calculated-fragment const., calculated- π const., Rekker 1977)

2.53; 2.65 (HPLC- k' correlation, Miyake & Terada 1982)

2.66 (electrometric titration, Clarke 1984)

2.72 (shake flask-OECD 1981 Guidelines., Geyer et al. 1984)

2.65 (centrifugal partition chromatography, Terada et al. 1987)

2.60; 2.67 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.67 (HPLC-RT correlation, Wang et al. 1989)

- 2.65 (HPLC-RT correlation, Hayward et al. 1990)
- 2.71 (countercurrent chromatography, average value, Vallat et al. 1990)
- 2.66 (centrifugal partition chromatography; El Tayar et al. 1991)
- 2.62 (shake flask-UV at pH 2, Da et al. 1992)
- 2.65 (recommended, Sangster 1994)
- 2.65 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

- < 1.0, 1.80, 2.23 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- 1.80, 1.99 (alga *chlorella fusca*, wet wt. basis, calculated- K_{OW} , Geyer et al. 1984)
- < 1.0, 1.78, 2.23 (golden ide, algae, activated sludge, Freitag et al. 1985)

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

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

Volatilization:

Photolysis:

Oxidation:

$k(aq.) \leq 0.15 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–6 and $22 \pm 1^\circ\text{C}$, with $t_{1/2} \geq 3 \text{ d}$ at pH 7 (Yao & Haag 1991).

Hydrolysis:

Biodegradation: decomposition by a soil microflora, $t_{1/2} = 64 \text{ d}$; degradation by waste water or soil suspension at pH 7.3 and 30°C , $t_{1/2} > 25 \text{ d}$ (quoted, Verschueren 1983).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} \geq 3 \text{ d}$ at pH 7 based on reaction rate with ozone in water (Yao & Haag 1991)

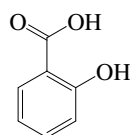
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.10 Salicylic acid



Common Name: Salicylic acid

Synonym: 2-hydroxybenzoic acid, *o*-hydroxybenzoic acid

Chemical Name: salicylic acid, 2-hydroxybenzoic acid

CAS Registry No: 69-72-7

Molecular Formula: $C_7H_6O_3$, HOC_6H_4COOH

Molecular Weight: 138.121

Melting Point ($^{\circ}C$):

159.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

256 (Verschuereen 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.443 (Weast 1982–83; Verschuereen 1983)

Molar Volume (cm^3/mol):

95.7 ($20^{\circ}C$, calculated-density)

147.4 ($158.6^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

3.009 (Korman & La Mer 1936)

3.52 ± 0.03 (HPLC, Unger et al. 1978)

3.29 ± 0.03 (HPLC, Unger et al. 1978)

2.96 (equilibrium titration, Clarke & Cahoon 1987)

2.97 (Sangster 1993)

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

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0484 (mp at $159^{\circ}C$)

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

5570* ($50^{\circ}C$, synthetic method, measured range 50 – $159^{\circ}C$, critical solution temp. $89.5^{\circ}C$, Sidgwick & Ewbank 1921)

1840* ($20^{\circ}C$, synthetic method, measured, range 10 – $87^{\circ}C$, Bailey 1925)

1800 ($20^{\circ}C$, Hodgman 1952; Verschuereen 1983)

1550 (shake flask-UV, Yalkowsky et al. 1983)

2555* (shake flask-TN, measured range 283.15 – $339.15 K$, Apelblat & Manzurola 1989)

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

133.3* ($113.7^{\circ}C$, summary of literature data, temp range 113.7 – $159^{\circ}C$, Stull 1947)

30.93* ($95.20^{\circ}C$, transpiration method, measured range 95.2 – $134.96^{\circ}C$, Davies & Jones 1954)

$\log(P/mmHg) = 12.8585 - 4968.7/(T/K)$, temp range 70.48 – $114.11^{\circ}C$ (transpiration, Davies & Jones 1954)

$\log(P/mmHg) = [-0.2185 \times 18920.7/(T/K)] + 10.822961$; temp range 113.7 – $256.0^{\circ}C$ (Antoine eq., Weast 1972–73)

2.85 ($70.5^{\circ}C$, effusion method, DePablo 1976)

0.0208 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.9834 - 4968.7/(T/K)$; temp range 368 – $408 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.53812 - 1049.95/(-228.144 + T/K)$; temp range 445 – $504 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$$\log(P/\text{mmHg}) = 177.3858 - 1.2871 \times 10^4/(T/K) - 56.301 \cdot \log(T/K) - 1.6667 \times 10^{-7} \cdot (T/K) + 1.1353 \times 10^{-5} \cdot (T/K)^2;$$

temp range 432–739 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.00144 (calculated-P/C)

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

- 2.26 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1971)
- 2.21 (shake flask, unpublished result, Leo et al. 1971)
- 2.24 (shake flask, pH 2, Korenman 1975)
- 2.38 (shake flask-UV, Tomida et al. 1978)
- 2.00 ± 0.01 , 2.18 ± 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.26, 2.21, 2.24, 2.25, 0.95 (quoted lit. values; Hansch & Leo 1979)
- 1.90 (HPLC-RT correlation, Butte et al. 1981)
- 2.25 ± 0.03 (exptl.-ALPM, Garst & Wilson 1984)
- 1.13, 1.92 (HPLC- k' correlation, Haky & Young 1984)
- 2.21 (shake flask-HPLC at pH 2, Bundgaard et al. 1986; Bundgaard & Nielsen 1988)
- 2.34 (electrometric titration, Clarke & Cahoon 1987)
- 2.24 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.08 (RP-TLC retention time correlation, Jack et al. 1988)
- 0.78 (shake flask-UV, Kuban 1991)
- 2.64 (centrifugal partition chromatography, Ilchmann et al. 1993)
- 2.26 (recommended, Sangster 1993)
- 2.11 (recommended, pH 7.4, Hansch et al. 1995)
- 1.70 (pH 7.0), -0.90 (pH 7.4); 2.26 (literature values; Hansch et al. 1995)
- 2.02 (shake flask-micro-volume liquid-liquid flow extraction system, Carlsson & Karlberg 2000)
- 1.44 (shake flask, buffered with 20 mM phosphate buffer pH 7.4, Carlsson & Karlberg 2000)

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

Bioconcentration Factor, $\log \text{BCF}$:

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

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

Volatilization:

Photolysis:

Oxidation: rate constants $k < 600 \text{ M}^{-1} \text{ s}^{-1}$ at pH 1.3–3, $k = (30 \pm 10) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4–7 using 4 mM *t*-BuOH as scavenger for the reaction with ozone in water and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983a);

rate constants $k < 500 \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, $k = (2.8 \pm 3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 4 mM *t*-BuOH as scavenger at pH 1.5–7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b).

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983);

average rate of biodegradation $95.0 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:
Biota:

TABLE 13.1.2.10.1
Reported aqueous solubilities of salicylic acid at various temperatures

Sidgwick & Ewbank 1921		Bailey 1925		Apelblat & Manzurola 1989	
synthetic method		synthetic method		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
50.0	5570	10	1310	283.15	1533
56.0	7170	20	1840	298.15	2555
80.0	20260	30	2610	307.15	3385
97.9	52700	40	3950	317.15	4393
101.4	80200	50	5920	318.15	5196
105.6	168200	60	8640	320.15	5156
106.7	340200			323.15	5697
107.2	488180			324.15	6027
109.5	65400			325.15	6502
119.5	80000			327.15	7166
131.8	89750			328.15	7401
159.0	100000			330.65	8502
				334.65	10021
				339.15	11433
critical solution temp 89.5°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$ for temp range 288–313 K	

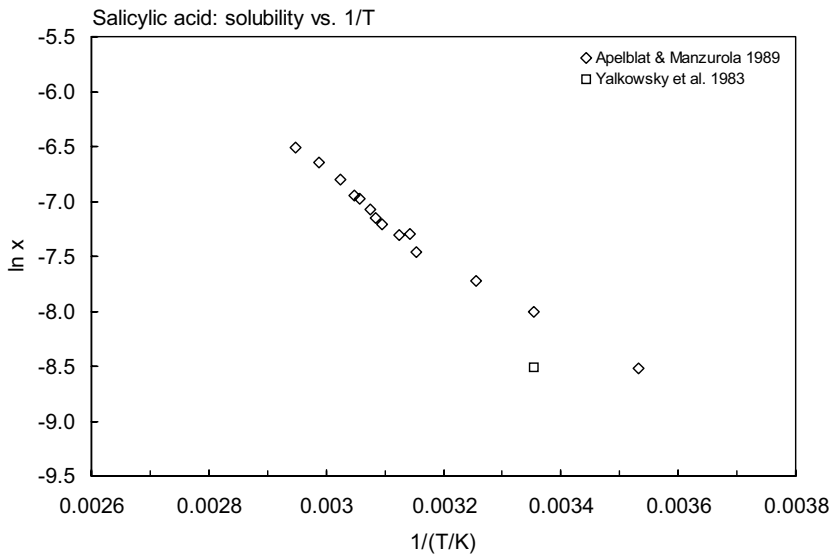


FIGURE 13.1.2.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for salicylic acid.

TABLE 13.1.2.10.2

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

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

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

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

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Davies & Jones 1954	
summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
113.7	133.3	95.20	30.93
136.0	666.6	100.49	48.66
146.2	1333	105.18	70.79
156.8	2666	109.96	103.7
172.2	5333	115.01	153.3
182.0	7999	119.98	220.4
193.4	13332	125.13	322.9
210.0	26664	134.96	649.3
230.5	53329		
256.0	101325	mp/°C	158.0–158.6
mp/°C	159	eq. 1	P/mmHg
		A	12.8585
		B	4968.7
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.144$			

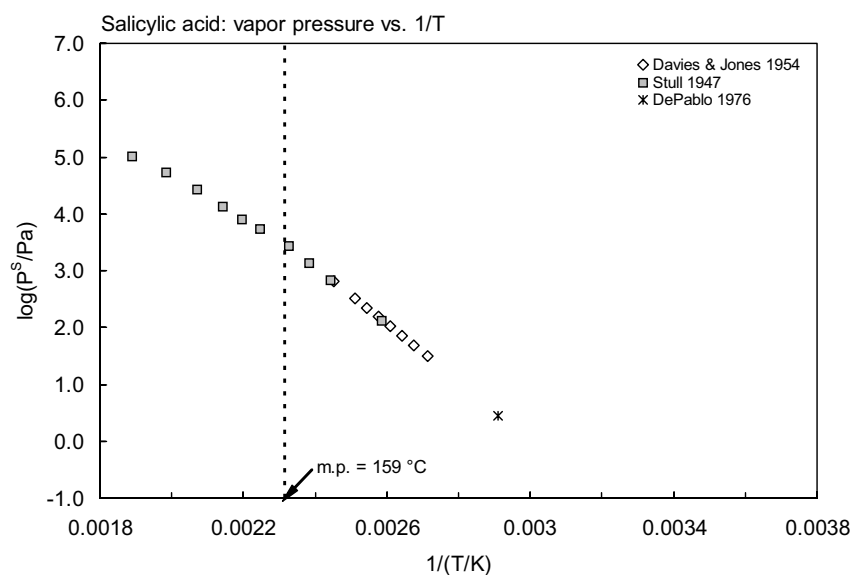
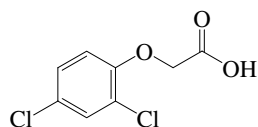


FIGURE 13.1.2.10.2 Logarithm of vapor pressure versus reciprocal temperature for salicylic acid.

13.1.2.11 2,4-Dichlorophenoxyacetic acid (2,4-D) (See also [Chapter 17](#), Herbicides)

Common Name: 2,4-Dichlorophenoxyacetic acid

Synonym: 2,4-D

Chemical Name: 2,4-dichlorophenoxyacetic acid

CAS Registry No: 94-75-7

Molecular Formula: $C_8H_6Cl_2O_3$, $Cl_2C_6H_3OCH_2COOH$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

140.5 (Hartley & Kidd 1987; Howard 1991; Lide 2003)

Boiling Point ($^{\circ}C$):

160 (at 0.4 mmHg, Dean 1985; Howard 1991)

215 (Neely & Blau 1985)

Density (g/cm^3 at $30^{\circ}C$):

1.565 (Neely & Blau 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

2.77 (potentiometric, Nelson & Faust 1969)

2.87 (spectrophotometric, Cessna & Grover 1978)

2.80 (Reinert & Rogers 1984)

2.64–3.31 (Howard 1991)

2.80 (selected, Wauchope et al. 1992)

2.97 (Sangster 1993)

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

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0736 (mp at $140.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

522 (shake flask-UV, Leopold et al. 1960)

725 (Bailey & White et al. 1965)

725, 400, 900, 550 (review, Günther et al. 1968)

890 (Hamaker 1975)

900 (Kenaga 1980a,b; Kenaga & Goring 1980)

600 ($20^{\circ}C$, Khan 1980)

470 (20 – $25^{\circ}C$, pH 5.6, Geyer et al. 1981)

633, 812 (15, $25^{\circ}C$, shake flask method, average values of 5 laboratories, OECD 1981)

620 ($20^{\circ}C$, Kidd & Hartley 1987; Worthing 1983)

609 (Gerstl & Helling 1987)

682 (Yalkowsky et al. 1987; quoted, Howard 1991)

703 (Gustafson 1989)

900, 600, 890, 703, 1072 (quoted, Wauchope et al. 1992)

890 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.0×10^{-5} (Hamaker 1975)

0.180–1.69 (transpiration method, Spencer 1976)

53.0 ($160^{\circ}C$, Kidd & Hartley 1983, 1987)

8.0×10^{-5} (recommended, Neely & Blau 1985; Lyman 1985)

1.00 ($20^{\circ}C$, selected, Suntio et al. 1988)

- 0.0032 (estimated from Henry's law constant, Howard 1991)
 5.6×10^{-5} (selected, Mackay & Stiver 1991)
 1.3×10^{-5} , 8.0×10^{-5} , 1.07×10^{-3} (quoted, Wauchope et al. 1992)
0.00107 (20–25°C, selected, Wauchope et al. 1992)

Henry's Law Constant (Pa·m³/mol):

- 0.55 (calculated-P/C, Suntio et al. 1988)
 1.03×10^{-3} (calculated-bond contribution, Howard 1991)

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

- 2.81 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
2.59 (electrometric titration, Freese et al. 1979)
1.57 (Kenaga & Goring 1980, Kenaga 1980b)
1.57, 4.88 (shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
−1.36 (Gerstl & Helling 1987)
2.65 (shake flask, Hansch & Leo 1987)
2.65 (centrifugal chromatography, Ilchmann et al. 1993)
2.81 (recommended, Sangster 1993)
2.81 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.11, −0.097 (calculated-S, K_{OW}, Kenaga 1980a)
−2.46, 1.30 (beef fat, fish, Kenaga 1980b)
0.778, 1.94 (alga *Chlorella fusca*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
0.778, < 1.0, 1.23 (algae, golden orfe, activated sludge, Freitag et al. 1982)
0.00 (fish, microcosm conditions, Garten & Trabalka 1983)
0.778, 1.23 (algae, calculated-K_{OW}, Geyer et al. 1984)
1.11 (calculated, Isensee 1991)
−5.0 (bluegill sunfish and channel catfish, Howard 1991)
−2.70 (frog tadpoles, Howard 1991)
−3.0, −2.52 (pH 7.8, seaweeds, Howard 1991)
0.778, 0.85 (quoted: alga, fish, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
1.30, 2.11 (quoted, Kenaga & Goring 1980)
1.68, 1.86, 1.68; 1.76 (commerce soil, Tracy soil, Catlin soil; average value of 3 soils, McCall et al. 1981)
2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
1.29 (soil, Neely & Blau 1985)
1.61 (soil, quoted, Sabljic 1987)
1.75, 2.00 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
1.29–2.13 (soil, quoted values, Howard 1991)
1.30 (selected, Mackay & Stiver 1991)
1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted, Wauchope et al. 1992)
1.30 (soil, selected, Wauchope et al. 1992)
0.68 (calculated-K_{OW}, Kollig 1993)

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

- Volatilization: volatilization from water is negligible, calculated volatilization t_{1/2} = 660 d from soil of 1 cm deep and t_{1/2} = 7.1 yr from 10 cm deep (Howard 1991).
Photolysis: aqueous photolysis t_{1/2} = 2–4 d when irradiated at 356 nm, t_{1/2} = 50 min in water when irradiated at 254 nm, and t_{1/2} = 29–43 d when exposed to September sunlight (Howard 1991).

Oxidation: photooxidation $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at $\text{pH} > 8$ (Howard 1991).

Biodegradation: degradation kinetics not first-order, time for 50% decomposition in six soils: $t_{1/2} = 5$ d in Commerce soil, $t_{1/2} = 1.5$ d in Catlin soil, $t_{1/2} = 3.9$ d in Keith soil, $t_{1/2} = 3.0$ d in Cecil soil, $t_{1/2} = 2.5$ d in Walla-Walla soil and $t_{1/2} = 8.5$ d in Fargo soil, with an average time of 4 d (McCall et al. 1981);

easily degraded under aerobic conditions with $t_{1/2} = 1.8$ and 3.1 d for cometabolism and metabolism respectively, under anaerobic conditions the degradation rate decreases and the $t_{1/2} = 69$ and 135 d (Liu et al. 1981; quoted, Muir 1991);

second-order $k = (3.6\text{--}28.8) \times 10^{-6} \text{ mL cell}^{-1} \text{ d}^{-1}$ in natural water (Paris et al. 1981; quoted, Klečka 1985);

first-order $k < 0.14\text{--}0.07 \text{ d}^{-1}$ in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985);

$k = 0.058 \pm 0.006 \text{ d}^{-1}$ in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985; quoted, Muir 1991);

$k = 0.08\text{--}0.46 \text{ d}^{-1}$ in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 240\text{--}1200$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980a, b; quoted, Howard et al. 1991; Muir 1991);

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}4320$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

first-order $k = 0.035 \text{ d}^{-1}$ in die-away test, $k = 0.029 \text{ d}^{-1}$ in CO_2 evolution test in soil and $k = 6.9 \times 10^{-1} \text{ mL} \cdot (\text{g bacteria})^{-1} \cdot \text{d}^{-1}$ by activated sludge cultures (Scow 1982);

biodegradation $t_{1/2} = 18$ to > 50 d in clear river water and $t_{1/2} = 10$ to 25 d in muddy water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to $t_{1/2} = 1.8\text{--}3.1$ d under aerobic conditions and $t_{1/2} = 69\text{--}135$ d under anaerobic conditions (Howard 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photooxidation $t_{1/2} = 23.9$ h for reactions with hydroxyl radicals in air (Howard 1991).

Surface water: $t_{1/2} = 48\text{--}96$ h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Howard et al. 1991);

degradation $t_{1/2} = 14$ d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of $1 \mu\text{g mL}^{-1}$ in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

typical biodegradation $t_{1/2} = 10$ to < 50 d with longer expected in oligotrophic waters, photolysis $t_{1/2} = 29\text{--}43$ d for water solutions irradiated at sunlight (Howard 1991).

Groundwater: $t_{1/2} = 480\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991).

Soil: $t_{1/2} = 240\text{--}1200$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

biodegradation $t_{1/2} < 1$ d to several weeks, $t_{1/2} = 3.9$ and 11.5 d in 2 moist soils and $t_{1/2} = 9.4$ to 254 d in the same soils under dry conditions (Howard 1991);

field $t_{1/2} = 2\text{--}16$ d, with a selected value of 10 d (Wauchope et al. 1992).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).

13.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 13.2.1

Summary of physical properties of carboxylic acids

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm³/mol		pK _a
							MW/ρ at 20°C	Le Bas	
Aliphatics:									
Formic acid	64-18-6	HCOOH	46.026	8.3	101	1	37.91	46.2	3.75
Acetic acid	64-19-7	CH ₃ COOH	60.052	16.64	117.9	1	57.24	68.4	4.75
Propionic acid	79-09-4	C ₂ H ₅ COOH	74.079	−20.5	141.15	1	74.60	90.6	4.87
Butyric acid	107-92-6	C ₃ H ₇ COOH	88.106	−5.1	163.75	1	92.00	112.8	4.82
Isobutyric acid	79-31-2	(CH ₃) ₂ CHCOOH	88.106	−46	154.45	1	91.00	112.8	4.86
<i>n</i> -Valeric acid	109-52-4	C ₄ H ₉ COOH	102.132	−33.6	186.1	1	108.77	135.0	4.83
3-Methylbutanoic acid	503-74-2	C ₅ H ₁₀ O ₂	102.132	−29.3	176.5	1	109.70	135.0	4.777
Trimethylacetic acid	75-98-9	(CH ₃) ₃ CCOOH	102.132	35	164	0.798		135.0	4.81
Hexanoic acid (Caproic acid)	142-62-1	C ₅ H ₁₁ COOH	116.158	−3	205.2	1	125.79	157.2	4.87
Octanoic acid	124-07-2	C ₇ H ₁₅ COOH	144.212	16.5	239	1		201.6	4.85
Stearic acid	57-11-4	C ₁₇ H ₃₅ COOH	284.478	69.3	350 dec	0.368	302.38	423.6	4.5
Oleic acid	112-80-1	C ₁₈ H ₃₄ O ₂	282.462	13.4	360	1	316.13	416.2	
Acrylic acid (2-Propenoic acid)	79-10-7	CH ₂ =CHCOOH	72.063	12.5	141	1	68.56	83.2	4.255
2-Butenoic (<i>cis</i> -)	503-64-0	CH ₃ CH=CHCOOH	86.090	15	169	1	83.85	105.4	4.5
2-Butenoic (<i>trans</i> -)	107-93-7	CH ₃ CH=CHCOOH	86.090	71.5	184.7	0.350		105.4	
Vinylacetic acid	625-38-7	CH ₂ =CHCH ₂ COOH	86.090	−35	169	1	85.31	105.4	4.35
2-Methylpropenoic acid	79-41-4	C ₄ H ₆ O ₂	86.090	16	162.5	1	84.79	105.4	4.66
Chloroacetic acid	79-11-8	ClCH ₂ COOH	94.497	63	189.3	0.424	67.29	89.3	2.85
Dichloroacetic acid	79-43-6	Cl ₂ CHCOOH	128.942	13.5	194	1	82.48	110.2	1.26
Trichloroacetic acid	76-03-9	Cl ₃ CCOOH	163.387	59.2	196.5	0.462	100.86	131.1	0.7
Aromatics:									
Benzoic acid	65-85-0	C ₆ H ₅ COOH	122.122	122.35	249.2	0.111		134.8	4.19
2-Methylbenzoic acid	118-90-1	CH ₃ C ₆ H ₄ COOH	136.149	103.5	259	0.170		157.0	3.91
3-Methylbenzoic acid	99-04-7	CH ₃ C ₆ H ₄ COOH	136.149	109.9	263	0.147		157.0	4.27
4-Methylbenzoic acid	99-94-5	CH ₃ C ₆ H ₄ COOH	136.149	179.6	275	0.0304		157.0	4.39
Phenylacetic acid	103-82-2	C ₆ H ₅ CH ₂ COOH	136.149	76.5	265.5	0.312	125.95	157.0	4.31
Phthalic acid	88-99-3	C ₆ H ₄ .1,2-(COOH) ₂	166.132	230 dec	dec	0.00974	104.29	173.6	
2-Chlorobenzoic acid	118-91-2	ClC ₆ H ₄ COOH	156.567	140.2	sublim	0.0741	101.4	155.7	

3-Chlorobenzoic acid	535-80-8	$\text{ClC}_6\text{H}_4\text{COOH}$	156.567	158	sublim	0.0496		155.7	3.82
4-Chlorobenzoic acid	74-11-3	$\text{ClC}_6\text{H}_4\text{COOH}$	156.567	243		0.00726		155.7	3.85
Salicylic acid	69-72-7	$\text{HOC}_6\text{H}_4\text{COOH}$	138.121	159		0.0484	95.72	142.2	2.97
Phenoxyacetic acid	122-59-8	$\text{C}_6\text{H}_5\text{OCH}_2\text{COOH}$	152.148	98.5	285 dec	0.190		164.4	
2,4-Dichlorophenoxyacetic acid	94-75-7	$\text{Cl}_2\text{C}_6\text{H}_3\text{OCH}_2\text{COOH}$	221.038	140.5	215	0.0736		206.2	
2,4,5-Trichlorophenoxyacetic acid	93-76-5	$\text{Cl}_3\text{C}_6\text{H}_2\text{OCH}_2\text{COOH}$	255.483	153	dec	0.0555		227.1	

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 13.2.2
Summary of selected physical-chemical properties of carboxylic acids at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol)		
	Solubility			Vapor pressure		log K _{ow}	calcd P/C	exptl ^a	calcd ^b
	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)	P ^S /Pa	P _L /Pa				
Aliphatics:									
Formic acid	miscible			5750	5750	−0.54		0.01832	
Acetic acid	miscible			2079	2079	−0.31		0.01825	0.0285
Propionic acid	miscible			435	435	0.26		0.018	0.0431
Butyric acid	miscible			84	84	0.79		0.0222	0.0650
Isobutyric acid	22800	258.8	258.8	185	185	0.79	0.715	0.0897	
<i>n</i> -Valeric acid	24000	235.0	235.0	19	19	1.39	0.081	0.0478	0.099
3-Methylbutanoic acid	4100	40.14	40.14	25	25		0.623	0.0844	
Hexanoic acid	9580	82.47	82.47	5	5	1.92	0.0606	0.0768	0.149
Octanoic acid	79.8	0.553	0.553	3.72	3.72		6.723		0.338
Stearic acid	340	1.195	3.248		1.69 × 10 ^{−6}	8.23			
Oleic acid				0.00113	0.00113	7.64			
Acrylic acid	miscible			550	550	0.43			
2-Methylpropenoic acid	8900	103.4	103.4	100	100	0.93	0.9673		
Chloroacetic acid	miscible				18.5	0.22			
Dichloroacetic acid	miscible			35	35	0.92			
Trichloroacetic acid					11	1.33			
Aromatics:									
Benzoic acid	3400	27.84	250.8	0.11	0.991	1.89	3.95 × 10 ^{−3}		
2-Methylbenzoic acid	1074	7.888	46.40			2.46			
3-Methyl benzoic acid	1246	9.152	62.26	1.39	9.456	2.37	0.1512		
4-Methylbenzoic acid	331	2.431	79.97			2.34			
Phenylacetic acid	16600	121.9	390.8	0.83	2.660	1.41	6.81 × 10 ^{−3}		
Phthalic acid	7000	42.14	4326			0.73			
2-Chlorobenzoic acid	2100	13.41	181.0			1.99			
3-Chlorobenzoic acid	400	2.555	51.51			2.60			
4-Chlorobenzoic acid	70	0.4471	61.58			2.65			
Salicylic acid	2300	16.65	344.0	0.0208	0.440	2.20	1.25 × 10 ^{−3}		
Phenoxyacetic acid	12000	78.87	415.1			2.81			
2,4-D	890	4.026	54.71	8.0 × 10 ^{−5}	0.001	2.65	1.99 × 10 ^{−5}		
2,4,5-T	278	1.088	19.61						

^a Brimblecombe et al. 1992; ^b Hine & Mookerjee 1975.

TABLE 13.2.3

Suggested half-life classes for carboxylic acids in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatics:				
Formic acid	4	3	4	5
Acetic acid	3	3	4	5
Butyric acid	3	3	4	5
Hexanoic acid (Caproic acid)	3	3	4	5
Stearic acid (Octadecanoic acid)	3	3	4	5
Acrylic acid (2-Propenoic acid)	2	3	4	5
Vinylacetic acid	2	3	4	5
Chloroacetic acid	5	4	5	6
Aromatics:				
Benzoic acid	3	3	4	5
2-Methylbenzoic acid (<i>o</i> -Toluic acid)	3	3	4	5
Phenylacetic acid	3	3	4	5
Phthalic acid	3	3	4	5
2-Chlorobenzoic acid	4	5	6	7
Salicylic acid	3	3	4	5
2,4-Dichlorophenoxyacetic acid (2,4-D)	2	3	5	6
2,4,5-Trichlorophenoxyacetic acid (2,4,5-T)	3	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	<10
2	17 (~1 d)	10–30
3	55 (~2 d)	30–100
4	170 (~1 week)	100–300
5	550 (~3 weeks)	300–1,000
6	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 y)	10,000–30,000
9	~5 y	>30,000

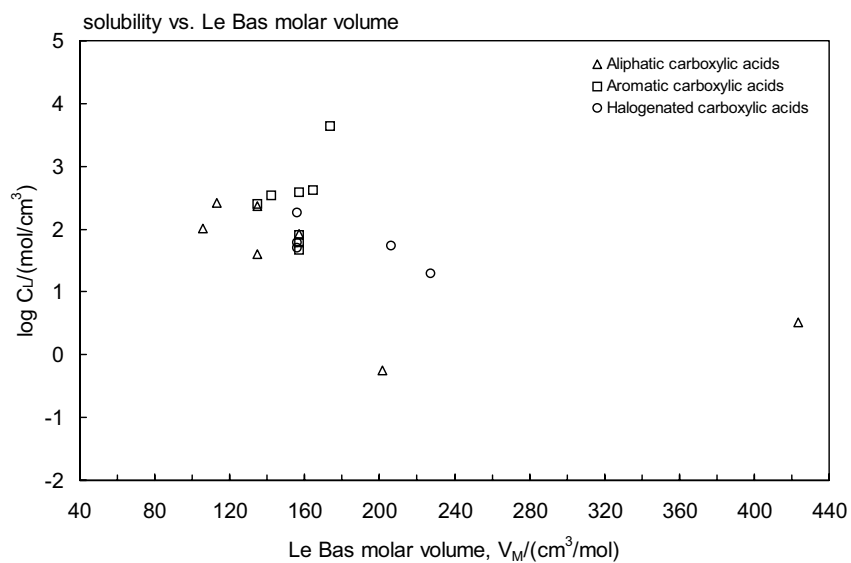


FIGURE 13.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

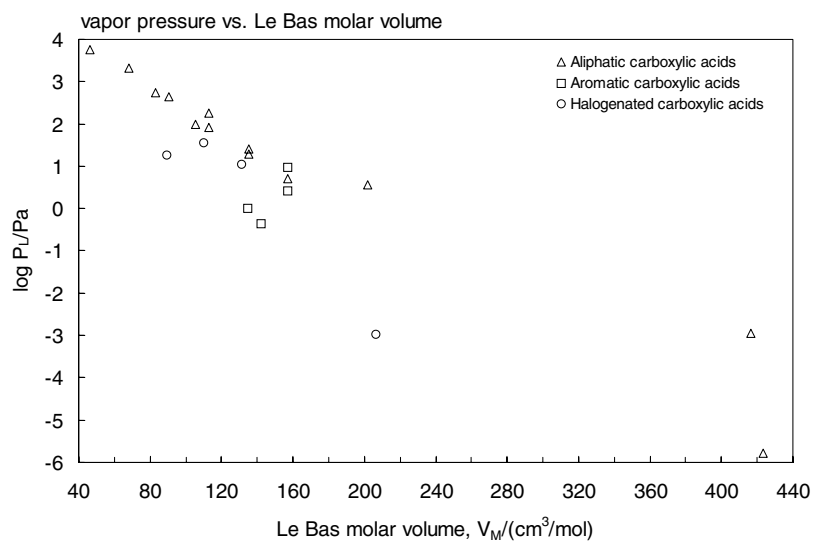


FIGURE 13.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

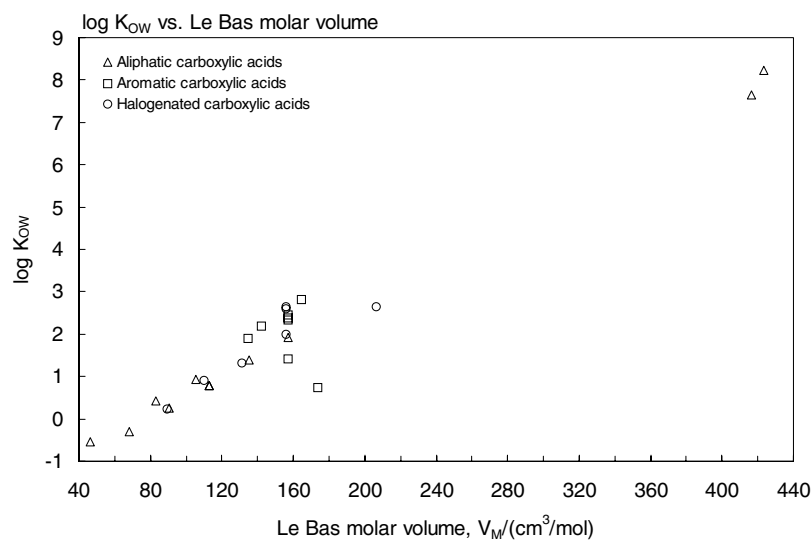


FIGURE 13.2.3 Octanol-water partition coefficient versus Le Bas molar volume for carboxylic acids.

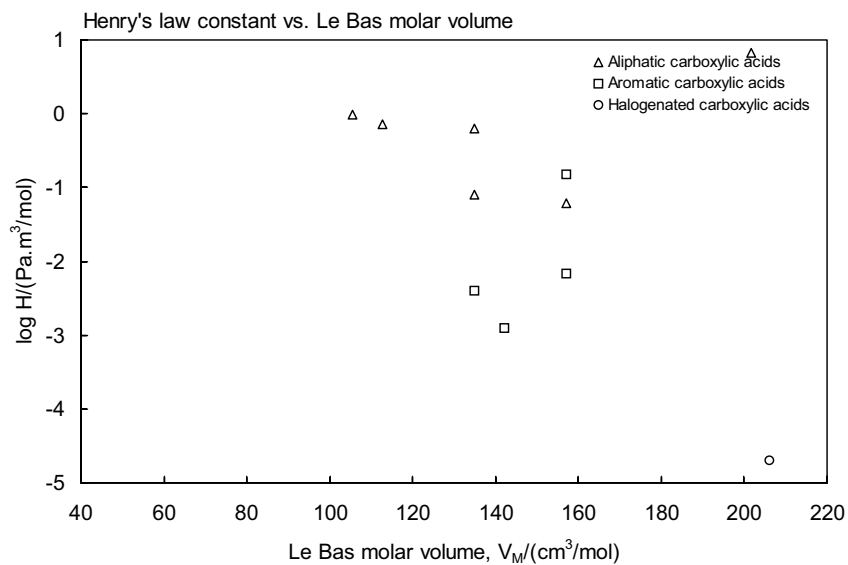


FIGURE 13.2.4 Henry's law constant versus Le Bas molar volume for carboxylic acids.

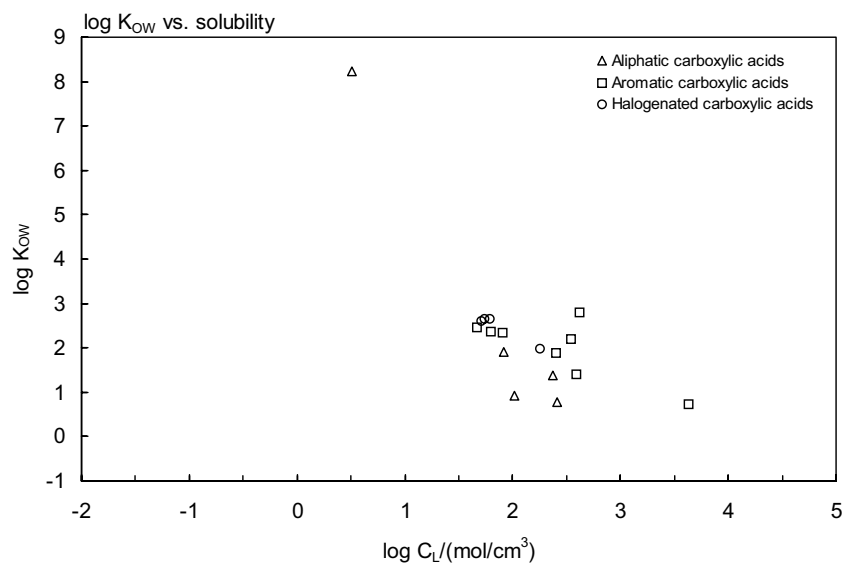


FIGURE 13.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for carboxylic acids.

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