12 Aldehydes and Ketones

CONTENTS

12.1   LIST OF CHEMICALS AND DATA COMPILATIONS

12.1.1   ALDEHYDES

12.1.1.1   Methanal (Formaldehyde)

Common Name: Formaldehyde
Synonym: formalin, methanal, oxomethane
Chemical Name: formaldehyde
CAS Registry No: 50-00-0
Molecular Formula: CH_2O, HCHO
Molecular Weight: 30.026
Melting Point (°C):
    –92.0   (Weast 1982–83; Dean 1985; Lide 2003)
Boiling Point (°C):
    –19.1   (Lide 2003)
Density (g/cm³):
    0.815   (–20°C, Weast 1982–83)
    0.815   (–20°C, Verschueren 1983; Dean 1985)
Molar Volume (cm³/mol):
    36.8   (–20°C, Stephenson & Malanowski 1987)
    29.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    1220000   (Dean 1985)
    very soluble, up to 55%   (Budavari 1989, Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    88566*   (–22.29°C, static method-differential manometer, measured range –109.39 to –22.29°C, Spencer & Wild 1935)
    101325*   (–19.5°C, summary of literature data, temp range –88 to –19.5°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 5917.9/(T/K)] + 7.985746; temp range –88 to –19.5°C (Antoine eq., Weast 1972–73)
    1333   (–88°C, Verschueren 1983)
    log (P/kPa) = 6.32524 – 972.5/(244.329 + t/°C), temp range (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    log (P/mmHg) = 7.1958 – 970.65/(244.1 + t/°C); temp range –109 to –22°C (Antoine eq., Dean 1985, 1992)
    log (P_L/kPa) = 6.5475 – 1062.4/(–19.92 + T/K), temp range 184–251 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.4306 – 1013.206/(–24.883 + T/K); temp range 163–251 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    517690   (1 atm, Howard 1989)
    log (P/mmHg) = 41.9603 – 2.1355 × 10³/(T/K) – 13.765·log (T/K) + 9.568 × 10⁻³·(T/K) – 5.1101 × 10⁻¹²·(T/K)²; temp range 181–408 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    0.0331   (20°C, porous membrane gas-liquid equilibration system, Dong & Dasgupta 1986)
    0.0169   (review, Gaffney et al. 1987)
    0.0341*   (gas stripping-headspace GC, measured range 15–45°C, Betterton & Hoffmann 1988)

0.0298*   (gas-stripping-HPLC-UV, freshwater, measured range 10–45°C, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –6.0 + 2844/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –6.7 + 3069/(T/K), temp range 25–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1‰), Zhou & Mopper 1990)

0.021   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_{AW} = 4.621 – 2840/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.35   (shake flask, Johnson & Piret 1948)
–1.54   (Kenaga & Goring 1980)
0.00   (Verschueren 1983)
0.35   (recommended, Sangster 1989)
0.35   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

no bioconcentration. in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis: sunlight photolysis $t_{1/2}$ = 1.25–6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991);

rate constant k = 8.0 × 10⁻⁵ s⁻¹ in the atmosphere (Carlier et al. 1986);

calculated lifetime of 4 h (Atkinson 2000).

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

k_{OH} = 1.4 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (discharge flow system-MS, Morris & Niki 1971)

aqueous photooxidation $t_{1/2}$ = 4813–190000 h, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; quoted, Howard et al. 1991)

k_{OH} = 1.5 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ (long-path Fourier transform IR, Niki et al. 1978)

k_{NO_3} = 3.2 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 ± 1 K (review, Atkinson & Lloyd 1984)

k = (0.1 ± 0.03) M⁻¹ s⁻¹ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

k_{HO_2} = 4.5 × 10⁻¹⁴ cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with HO₂ radical at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

k_{OH} = 1.1 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

k_{OH}(calc) = 7.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, k_{OH}(obs.) = 9.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1985)

atmospheric photooxidation half-life of 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

k_{OH}* = 9.77 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

k_{NO_3} = 5.8 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1991)

k_{OH}(calc) = 17.5 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

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

Biodegradation: degradation complete in 20 h under aerobic conditions and 48 h under anaerobic conditions in a die-away test using water from a stagnant lake (Howard 1989)

aqueous aerobic half-life of 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data; aqueous anaerobic half-life of 96–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environmental Compartments:

Air: half-life is a few hours in the sunlit troposphere; $t_{1/2}$ = 19 and 50 h by dry deposition and wet removal, respectively; $t_{1/2}$ = 12 d when reacts with NO_3 radical by H-atom abstraction. (Howard 1989)

photooxidation $t_{1/2}$ = 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

$t_{1/2}$ = 1.26–6.0 h, based on photolysis half-life in air (Howard et al. 1991);

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

calculated lifetimes of 1.2 d, 80 d and > 4.5 yr for reactions with OH radical, NO_3 radical and O_3, respectively (Atkinson 2000).

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

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

Sediment:

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

Biota:

TABLE 12.1.1.1.1

Reported vapor pressures of methanal (formaldehyde) at various temperatures and the coefficients for the vapor pressure equations

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

Spencer & Wild 1935		Stull 1947	
differential manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
−109.39	127	−88.0	1333
−104.39	237	−79.6	2666
−98.29	480	−70.6	5333
−95.19	647	−65.0	7999
−89.09	1157	−57.3	13332
−85.59	1633	−46.0	26664
−78.89	2802	−33.0	53329
−78.29	2946	−19.5	101325
−71.29	4720		
−68.55	6190	mp/°C	−92
−65.29	7859		
−64.59	8219		
−63.69	8693		
−55.79	14799		
−53.99	16625		
−49.29	21745		
−40.59	35544		
−39.09	38743		
−34.29	49182		
−28.39	66208		
−22.29	88566		

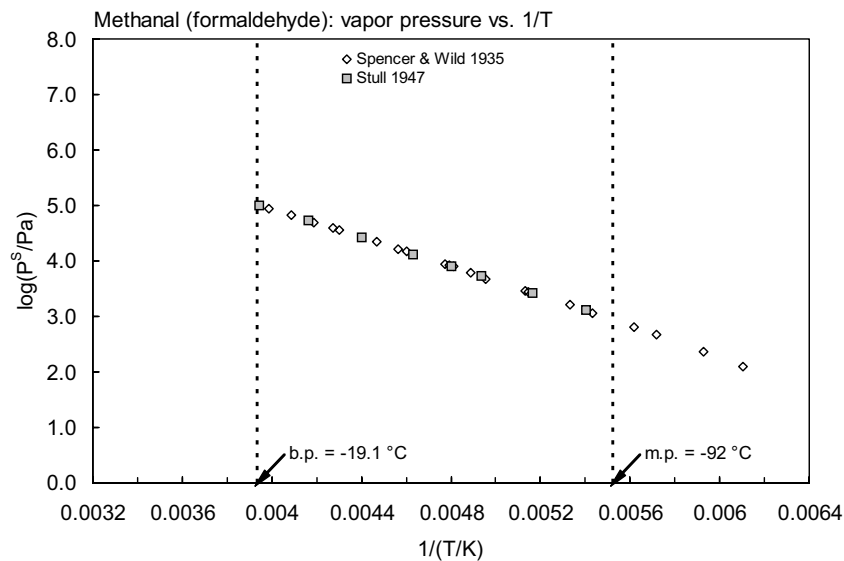Methanal (formaldehyde): vapor pressure vs. 1/T

FIGURE 12.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanal.

TABLE 12.1.1.1.2
Reported Henry's law constants of methanal (formaldehyde) at various temperatures and temperature dependence equations

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

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

$$\ln (k_H/atm) = A - B/(T/K) \quad (3)$$

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

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

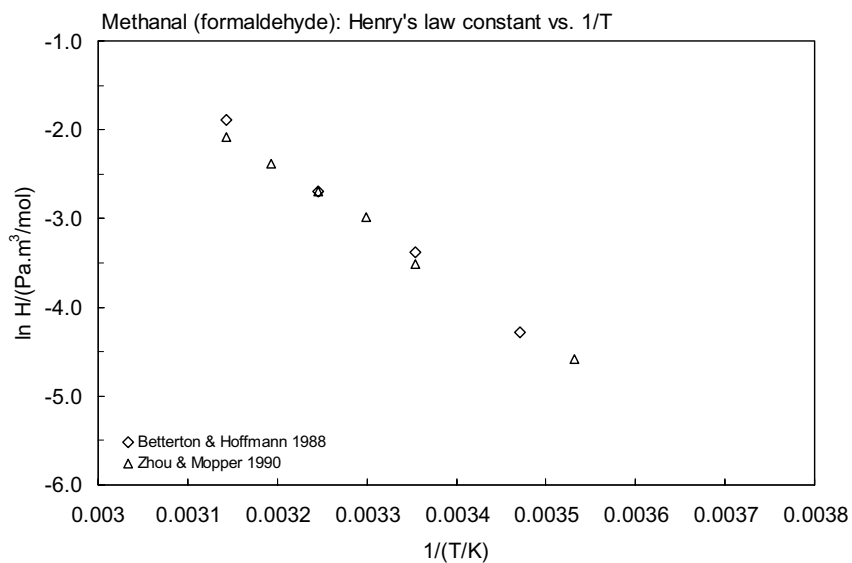| Betterton & Hoffmann 1988		Zhou & Mopper 1990			
gas stripping-fluorescence		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
		fresh water		sea water	
15	0.01386	10	0.01023	10	0.0074
15	0.01031*	17	-	17	0.0128
25	0.0341	25	0.0298	25	0.0284
35	0.0675	30	0.0507	30	0.0405
45	0.1506	35	0.0675	35	0.0533
		40	0.0921	40	-
$\Delta H/(kJ\ mol^{-1}) = -59.8$		45	0.125	45	0.115
* in 0.5 M HSO₄. solution		eq. 1a	$K_H'/(M/atm)$	eq. 1a	$K_H'/(M/atm)$
		A	−6.00	A	−6.70
		B	−2844	B	−3069

FIGURE 12.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanal.

12.1.1.2 Ethanal (Acetaldehyde)

Common Name: Acetaldehyde
Synonym: acetic aldehyde, aldehyde, ethanal, ethylaldehyde
Chemical Name: acetaldehyde, ethanal
CAS Registry No: 75-07-0
Molecular Formula: C_2H_4O, CH_3CHO
Molecular Weight: 44.052
Melting Point (°C):
    –123.37   (Lide 2003)
Boiling Point (°C):
    20.1   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7834   (18°C, Lide 2003)
Molar Volume (cm³/mol):
    56.23   (18°C, calculated-density)
    51.8   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    –10.2   (pK_b, Riddick et al. 1986)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    3.243   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    miscible   (Palit 1947; Riddick et al. 1986)
    miscible   (Verschueren 1983; Dean 1985)
    miscible   (Yaws et al. 1990)

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

    101300*   (20.2°C, summary of literature data, temp range –81.5 to 5.9°C, Stull 1947)
    102125*   (20.7°C, measured range –0.20 to 34.4°C, Coles & Popper 1950)
    120060   (Hoy 1970)
    $\log (P/mmHg) = [-0.2185 \times 7267.8/(T/K)] + 8.327803$; temp range –81.5 to 20.2°C (Antoine eq., Weast 1972–73)
    $\log (P/mmHg) = [-0.2185 \times 6622.1/(T/K)] + 7.82060$; temp range –24.3 to 27.5°C (Antoine eq., Weast 1972–73)
    98640   (20°C, Verschueren 1983)
    102125, 120220 (20.7°C, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)
    $\log (P/kPa) = 7.14122 - 1606.85/(292.482 + t/°C)$, temp range: –0.2 to 34.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    120230   (calculated-Antoine eq., Dean 1985, 1992)
    $\log (P/mmHg) = 8.00552 - 1600.017/(291.809 + t/°C)$, temp range: liquid (Antoine eq., Dean 1985, 1992)
    121300   (selected, Riddick et al. 1986)
    $\log (P/kPa) = 6.1814 - 1070.6/(236.0 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
    120700   (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 6.1410 - 1034.5/(-43.15 + T/K)$; temp range 272–294 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 6.03292 - 1012.828/(-41.823 + T/K)$; temp range 293–377 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    $\log (P/mmHg) = 87.3702 - 3.6822 \times 10^3/(T/K) - 31.548 \cdot \log (T/K) + 2.0114 \times 10^{-2} \cdot (T/K) + 5.5341 \times 10^{-13} \cdot (T/K)^2$; temp range 150–461 K (vapor pressure eq., Yaws 1994)

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

     6.692   (shake flask-concentration ratio-GC, Buttery et al. 1969)
     8.924   (calculated K_{AW}s, Buttery et al. 1969)
     6.672   (exptl., Hine & Mookerjee 1975)
     5.946, 5.423 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
     1.336, 8.0   (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
     6.75   (review, Gaffney et al. 1987)
     2.578*   (gas stripping-headspace GC, measured range 15–35°C, Betterton & Hoffmann 1988)
     6.80*   (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
     ln [K_H'/(M/atm)] = –6.03 + 276/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
     ln [K_H'/(M/atm)] = –5.21 + 1984/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1‰), Zhou & Mopper 1990)
     10.18   (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
     5.47*   (20°C, headspace-GC, measured range 10–40°C, Benkelberg et al. 1995)
     8.72*   (headspace-GC, artificial seawater, measured range 16–40°C, Benkelberg et al. 1995)
     ln (k_H/atm) = (20.4 ± 0.1) – (5671 ± 22)/(T/K); temp range 10–40°C (headspace-GC measurements, Benkelberg et al. 1995)
     5.14   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
     6.33   (solid-phase microextraction SPME-GC, Bartelt 1997)
     6.69   (equilibrium headspace-GC, Marin et al. 1999)
     5.39   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
     log K_{AW} = 5.324 – 2340/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

     0.52   (generator column-HPLC, Wasik et al. 1981)
     0.36   (generator column-GC, Tewari et al. 1982)
     0.43   (calculated, Verschueren 1983)
     0.45   (recommended, Sangster 1989, 1993)

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

Bioconcentration Factor, log BCF

Sorption Partition Coefficient, log K_{OC}:

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

     Volatilization:
     Photolysis: rate constant k = 2.3.0 × 10⁻⁵ s⁻¹ in the atmosphere (Carlier et al. 1986); calculated lifetime of 6 d (Atkinson 2000)
     Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and or Arrhenius equation see reference:
         k_{OH} = 1.53 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (discharge flow system-MS, Morris & Niki 1971)
         k_{OH} = 1.6.2 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ (long-path Fourier transform IR, Niki et al. 1978)
         k = 0.1 M⁻¹ s⁻¹ for oxidation by RO_2 radical at 30°C in aquatic systems with half-life of 8 × 10⁴ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
         k < 2 × 10² M⁻¹ s⁻¹ for oxidation by singlet oxygen at 25°C in aquatic systems with half-life > 00 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
         k_{OH} = (12.8 ± 4.3) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (Kerr & Sheppard 1981; quoted, Atkinson 1985)
         k = (1.5 ± 0.2) M⁻¹·s⁻¹ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)
         k_{OH} = (12.2 ± 2.7) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)
         k_{O3} = (3.4 ± 0.5) × 10⁻²⁰ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (Stedman & Niki 1973; quoted, Atkinson & Carter 1984)

$k_{OH} = 9.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (Lyman 1982)

$k_{O3} \leq 6 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} 296 ± 2 K (Atkinson et al. 1981, 1982; quoted, Atkinson & Carter 1984; Atkinson 1985)

$k_{HO2} = 1.0 \times 10^{-17}$ cm^3·molecule^{-1} s^{-1} for the gas-phase reaction with HO$_2$ radical at 293 K in the atmosphere (Barnes et al. 1982; quoted, Carlier et al. 1986)

$k_{OH} = 1.62 \times 10^{-11}$ cm^3·molecule^{-1} s^{-1}; and $k_{NO3} = 3.02 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K in air (Atkinson et al. 1984)

$k_{NO3} = 1.40 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} 298 ± 1 K (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{OH} = 1.60 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{OH} = (14.7 \pm 2.8) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Michael et al. 1985; quoted, Atkinson 1985)

k_{OH}(calc) $= 1.62 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) $= 1.62 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 1.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 0.7 d^{-1}, $k_{O3} \leq 6.0 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} with a loss rate of ≤ 0.0004 d^{-1}, $k_{NO3} = 2.5 \times 10^{-15}$ cm^3·molecule^{-1} s^{-1} with a loss rate of 0.05 d^{-1} (review, Atkinson 1985)

$k_{OH}* = 1.53 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 16.22 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 3.02 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{NO3} = 2.78 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

$k_{OH} = 10.64 \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

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

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

calculated lifetimes of 8.8 h, 17 d and > 4.5 yr for reactions with OH radical, NO$_3$ radical and O$_3$, respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.2.1
Reported vapor pressures of ethanal (acetaldehyde) at various temperatures and the coefficients for the vapor pressure equations

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

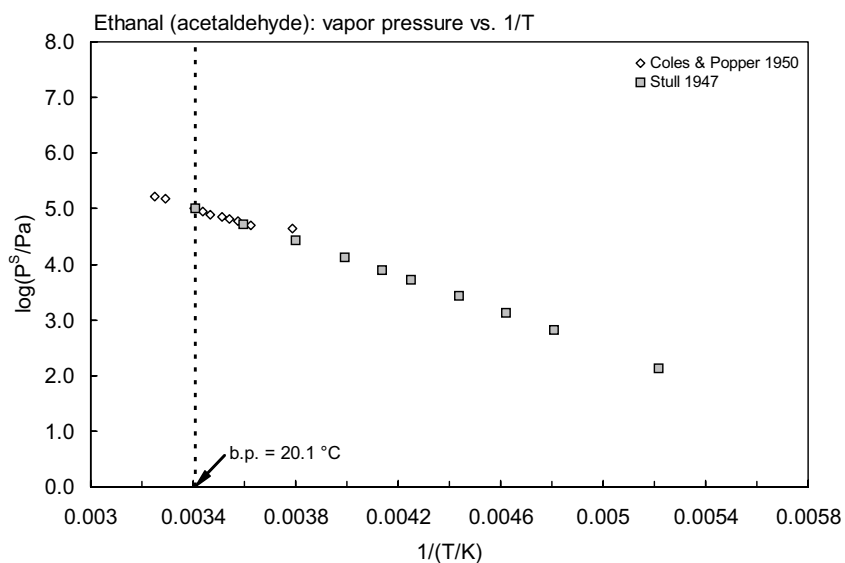| Stull 1947		Coles & Popper 1950	
summary of literature data		isoteniscope method	
t/°C	P/Pa	t/°C	P/Pa
−81.5	133.3	−0.20	44263
−65.1	666.6	2.70	49996
−56.8	1333	6.70	59062
−47.8	2666	9.30	65861
−37.8	5333	11.6	70794
−31.4	7999	15.3	76927
−22.6	13332	17.6	90926
−10.0	26664	20.7	102125
4.90	53329	30.8	149321
20.2	101325	34.4	167852
mp/°C	−123.5	bp/°C	20.4
		eq. 1	P/mmHg
		A	7.694
		B	1413

FIGURE 12.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethanal.

TABLE 12.1.1.2.2
Reported Henry's law constants of ethanal (acetaldehyde) at various temperatures and temperature dependence equations

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

1.

Snider & Dawson 1985		Betterton & Hoffmann 1988		Zhou & Mopper 1990			
gas stripping-GC		gas stripping-GC, spec.		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
					fresh water		sea water
0	1.336	5	1.829	10	2.277	10	3.147
25	8.00	10	2.578	17	-	17	5.170
		25	8.888	25	6.80	25	7.735
enthalpy of transfer:		35	15.446	30	8.238	30	9.296
ΔH/(kJ mol⁻¹) = −46.024				35	10.55	35	11.78
		ΔH/(kJ mol⁻¹) = −52.1		40	-	40	14.90
		at 25°C		45	15.59	45	17.78
				eq. 1a	$K_H'/(M/atm)$	eq. 1a	$K_H'/(M/atm)$
				A	−6.03	A	−5.21
				B	−2164	B	−1894

2.

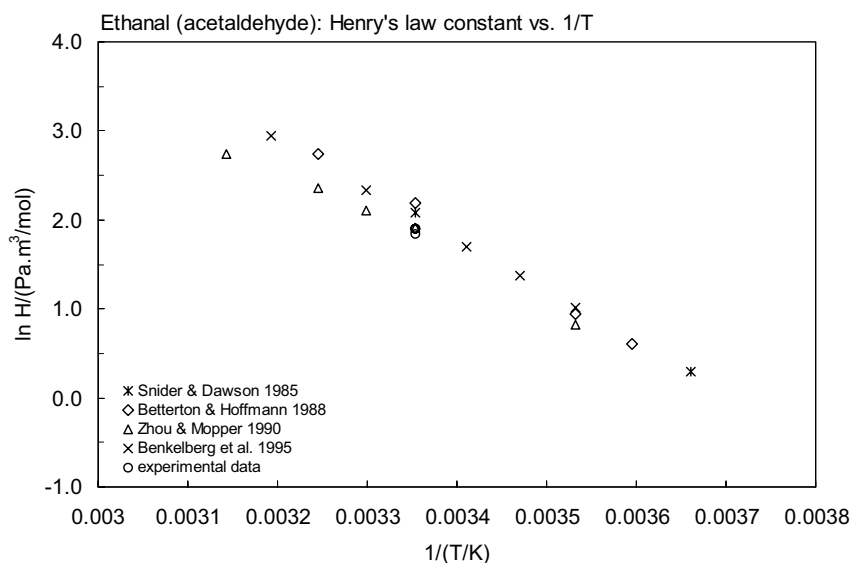| Benkelberg et al. 1995			
equilibrium vapor phase concentration-headspace GC			
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
	deionized water		artificial sea water
10	2.754	16	5.070
15	3.940	25	8.718
20	5.472	30	11.69
30	10.268	40	19.716
40	18.968		
for deionized and rain water:			
eq. 3	k_H/atm		
A	20.4 ± 0.1		
B	5671 ± 22		
ΔH/(kJ mol⁻¹) = −47.15			

FIGURE 12.1.1.2.2 Logarithm of Henry's law constant versus reciprocal temperature for ethanal.

12.1.1.3 Propanal (Propionaldehyde)
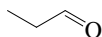
Common Name: Propionaldehyde
Synonym: propanal
Chemical Name: propionaldehyde, propanal
CAS Registry No: 123-38-6
Molecular Formula: C_3H_6O, CH_3CH_2CHO
Molecular Weight: 58.079
Melting Point (°C):
  –80   (Lide 2003)
Boiling Point (°C):
  48   (Lide 2003)
Density (g/cm³ at 20°C):
  0.8058   (Weast 1982–83)
  0.7970   (Riddick et al. 1986)
Molar Volume (cm³/mol):
  72.9   (calculated-density, Stephenson & Malanowski 1987)
  74.0   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  160000   (20°C, Seidell 1941)
  200000   (20°C, Verschueren 1983)
  306000   (Dean 1985; Riddick et al. 1986)
  405000   (selected, Yaws et al. 1990)
  310000*, 269000   (20°C, 30°C, shake flask-GC/TC, measured range 12.3–50°C, Stephenson 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  67661*   (39.07°C, ebulliometry, measured range 39.07–50.29°C, Dreisbach & Shrader 1949)
  $\log (P/\text{mmHg}) = 7.08683 – 1178.9/(230 + t/°C)$; temp range not specified (Antoine eq., Dreisbach & Martin 1949)
  42300*   (23°C, measured range 13.1–48.06°C, Ambrose & Sprake 1974)
  42340   (interpolated-Antoine eq., Boublik et al. 1984)
  $\log (P/\text{kPa}) = 6.2902 – 1210.87/(234.65 + t/°C)$, temp range 13.1–48.06°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1974, Boublik et al. 1984)
  42490, 42360   (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.2047 – 1166.99/(–43.15 + T/K)$; temp range 290–322 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.2336 – 1180/(–42.0 + T/K)$; temp range 250–330 K (Antoine eq.-II, Stephenson & Malanowski 1987)
  23190   (calculated-solvatochromic parameters, Banerjee et al. 1990)
  $\log (P/\text{mmHg}) = 26.1637 – 2.3059 \times 10^3/(T/K) – 6.5289 \cdot \log (T/K) – 2.3065 \times 10^{-10} \cdot (T/K) + 2.5454 \times 10^{-6} \cdot (T/K)^2$; temp range 193–496 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  7.436   (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
  7.486   (exptl., Hine & Mookerjee 1975)

8.40, 8.21   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

8.305*   (gas stripping-HPLC/UV, measured range 10–45°C, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –7.15 + 2467/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –6.60 + 2273/(T/K), temp range 25–35°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1l), Zhou & Mopper 1990)

7.486, 13.62 (quoted, correlated-molecular structure, Russell et al. 1992)

5.48   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_{AW} = 5.324 – 2237/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.83   (calculated, Verschueren 1983)

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

0.59   (recommended, Sangster 1989)

0.59   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis: rate constant k = 3.2×10^{-5} s^{-1} in the atmosphere (Carlier et al. 1986).

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

k_{OH} = 3.06×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (discharge flow system-MS, Morris & Niki 1971)

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

k_{OH} = 2.1×10^{-11} cm^3 molecule^{-1} s^{-1} (long-path Fourier transform IR, Niki et al. 1978)

k_{OH} = $(18.5 \pm 2.1) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Audley et al. 1981; quoted, Atkinson 1985),

k_{OH} = $(19.5 \pm 1.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Kerr & Sheppard 1981; quoted, Atkinson 1985)

k = (2.5 ± 0.4) M^{-1} s^{-1} for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

k_{OH} = 1.8×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

k_{OH} = $(17.1 \pm 2.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)

k_{OH}(calc) = 2.2×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.96×10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2}$ = 3.3–33 h in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991)

k_{OH} = 1.96×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 16.55×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

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

Biodegradation: biodegradation rate constants k = 0.046–0.063 h^{-1} in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b); aqueous aerobic $t_{1/2}$ = 24–168 h, based on aerobic biological screening test data (Gerhold & Malaney 1966; Dore et al. 1975; Urano & Kato 1986; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 96–672 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

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

photooxidation $t_{1/2}$ = 3.3–33 h in air, based on measured reaction rate constant for the vapor-phase reaction
   with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

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

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

Sediment:

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

Biota:

TABLE 12.1.1.3.1
Reported aqueous solubilities and vapor pressures of propanal (propionaldehyde) at various temperatures

| Aqueous solubility		Vapor pressure					
Stephenson 1993		Dreisbach & Shrader 1949		Dreisbach & Martin 1949		Ambrose & Sprake 1974	
shake flask-GC/TC		ebulliometry		ebulliometry		ebulliometry	
t/°C	S/g·m⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.3	477000	39.07	67661	data presented in		13.1	25300
15.6	368000	50.29	101325	log P = A − B/(C + t/°C)		23.0	42300
20.0	310000			eq. 2	P/mmHg	29.5	51000
30.0	269000			A	7.08683	47.95	101300
40.0	235000			B	1178.9	48.06	101700
50.0	197000			C	230		
				bp/°C	50.29		
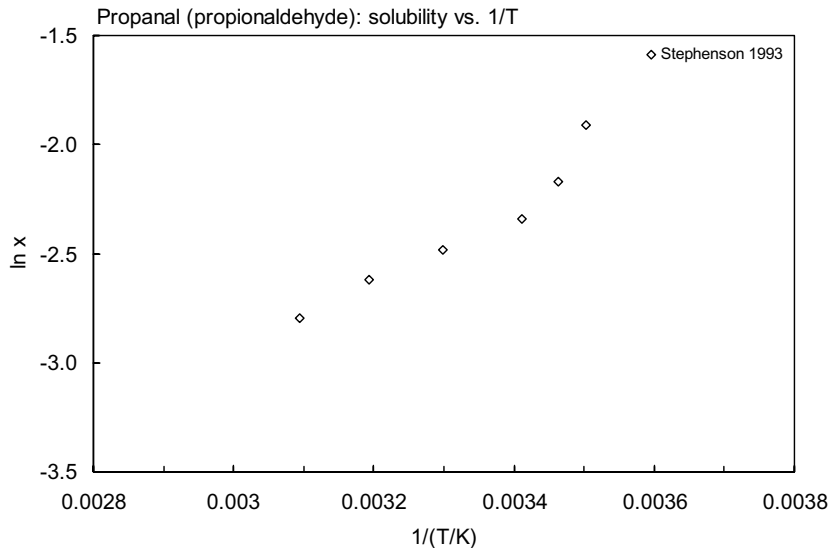
FIGURE 12.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for propanal.

TABLE 12.1.1.3.2

Reported Henry's law constants of propanal (propionaldehyde) at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \tag{1}$$

$$\ln (1/K_{AW}) = A - B/(T/K) \tag{2}$$

$$\ln (k_H/atm) = A - B/(T/K) \tag{3}$$

$$\ln [H/(Pa\ m^3/mol)] = A - B/(T/K) \tag{4}$$

$$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2 \tag{5}$$

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

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

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

Zhou & Mopper 1990

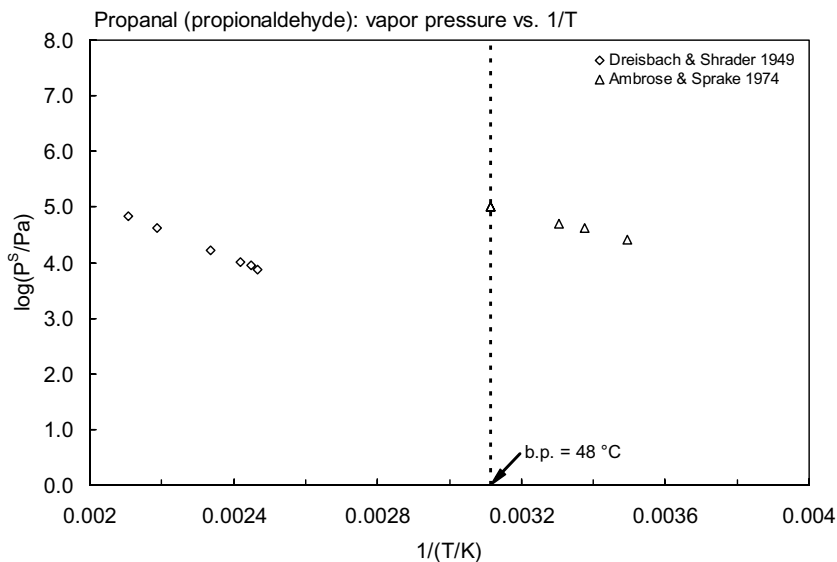| gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
fresh water		sea water	
10	2.605	10	3.389
17	-	17	6.495
25	8.305	25	10.13
30	10.67	30	12.67
35	14.07	35	16.34
40	-	40	22.03
45	23.56	45	28.15
eq. 1a	$K_H'/(M/atm)$	eq. 1a	$K_H'/(M/atm)$
A	−7.15	A	−6.60
B	−2467	B	−2273

FIGURE 12.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for propanal.
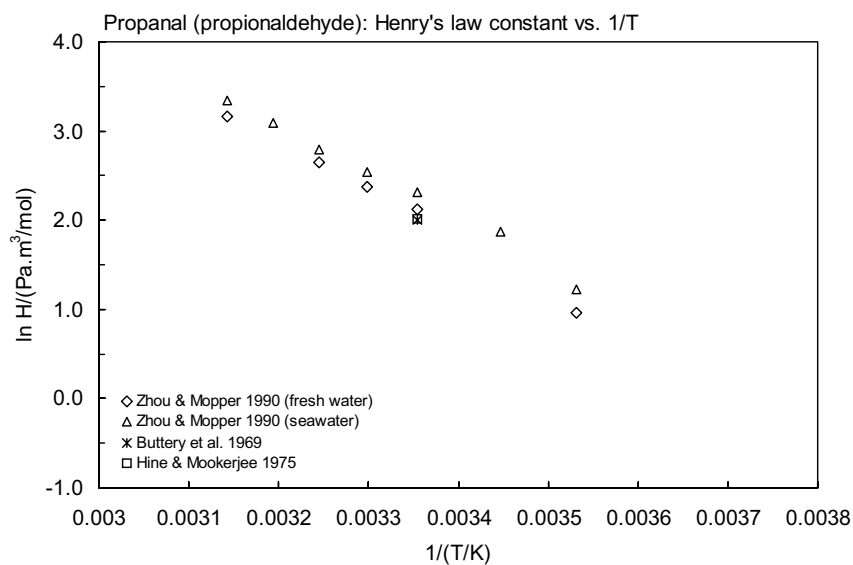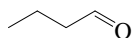
FIGURE 12.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for propanal.

12.1.1.4   Butanal (*n*-Butyraldehyde)

Common Name: *n*-Butyraldehyde
Synonym: 1-butanal, butylaldehyde, butyric aldehyde
Chemical Name: butyraldehyde, butanal
CAS Registry No: 123-72-8
Molecular Formula: C_4H_8O, $CH_3CH_2CH_2CHO$
Molecular Weight: 72.106
Melting Point (°C):
    –96.86   (Lide 2003)
Boiling Point (°C):
    74.8   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8170   (Weast 1982–83; Verschueren 1983)
    0.8016   (Dean 1985; Riddick et al. 1986)
Molar Volume (cm³/mol):
    90.0   (20°C, calculated-density)
    96.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    11.088   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    36000   (20°C, quoted, Palit 1947)
    37840   (Deno & Berkheimer 1960)
    37000, 71000   (lit. values, Verschueren 1983)
    71000   (Dean 1985; Riddick et al. 1986)
    83700   (selected, Yaws et al. 1990)
    74400*, 54800   (20°C, 30°C, shake flask-GC/TC, measured range 0–70°C, Stephenson 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    19372*   (30.71°C, measured range 30.71–74.03°C, Seprakova et al. 1959; quoted, Boublik et al. 1984)
    9464   (20°C, Verschueren 1983)
    14798   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.52728 – 921.802/(186.564 + t/°C); temp range 30.71–74.03°C (Antoine eq. from reported exptl. data of Seprakova et al. 1959, Boublik et al. 1984)
    14785   (extrapolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
    15700   (selected, Riddick et al. 1986)
    log (P/kPa) = 6.1461 – 1233.0/(223.0 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
    14780   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.68618 – 994.1/(–78.05 + T/K); temp range 293–349 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.40874 – 1182.472/(T/K); temp range 348–423 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = 66.8411 – 3.6784 × 10³/(T/K) –22.609·log (T/K) + 1.1697 × 10⁻²·(T/K) + 2.9647 × 10⁻¹³·(T/K)²; temp range 177–525 K (vapor pressure eq., Yaws 1994)

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

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

11.59, 11.594, 12.14 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

11.65   (gas stripping-HPLC, Zhou & Mopper 1990)

3.237, 11.65, 15.59, 20.68, 36.19 (10, 25, 30, 35, 45°C, gas-stripping-HPLC-UV, Zhou & Mopper 1990)

$\ln [K_H'/(M/atm)] = -8.07 + 2701/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/atm)] = -8.20 + 2698/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1l),. Zhou & Mopper 1990)

11.59, 11.59 (quoted, correlated-molecular structure, Russell et al. 1992)

7.26   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.244 - 2571/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.20   (Hansch & Leo 1979)

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

0.88   (recommended, Sangster 1989)

0.88   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis: rate constant $k = 2.7 \times 10^{-5}$ s⁻¹ in the atmosphere (Carlier et al. 1986)

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

photooxidation $t_{1/2}$ = 114 d to 19 yr in water, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (26.2 \pm 3.3) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Audley et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (25.3 \pm 0.6) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k_{OH} = 25 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k = (2.5 \pm 0.4)$ M⁻¹ s⁻¹ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (30.8 \pm 4.2) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (flash photolysis-resonance fluorescence technique. Semmes et al. 1985; quoted, Atkinson 1985)

$k_{OH}(calc) = 2.55 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(obs.) = 2.3 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2}$ = 2.8–28 h in air, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{OH}^* = 2.35 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: rate constants $k = 0.044$–0.069 h⁻¹ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b);

aqueous aerobic $t_{1/2}$ = 24–168 h, based on aerobic biological screening test data (Lamb & Jenkins 1952; Heukelekian & Rand 1955; Dore et al. 1975; Urano & Kato 1986b; selected, Howard et al. 1991);

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

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 2.8–28 h, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);

    calculated lifetimes of 5.9 d for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2}$ = 114 d to 19 yr, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991);

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

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

Sediment:

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

Biota:

TABLE 12.1.1.4.1
Reported aqueous solubilities and vapor pressures of butanal (*n*-butyraldehyde) at various temperatures

Aqueous solubility		Vapor pressure	
Stephenson 1993		Seprakova et al. 1959	
shake flask-GC/TC		in Boublik et al. 1984	
t/°C	S/g·m⁻³	t/°C	P/Pa
0	118200	30.71	19372
10.0	91200	38.36	26771
20.0	74400	43.93	33584
30.0	54800	48.33	39997
40.0	47100	52.36	46663
50.0	42500	55.90	53329
60.0	41700	62.29	66661
70.0	38900	67.73	79993
		74.03	97512
bp/°C	75		

eq in Boublik et al. 1984

$\log P = A - B/(C + t/°C)$

eq. 2	P/kPa
A	5.52728
B	921.802
C	186.564
bp/°C	75.195

Butanal (*n*-butyraldehyde): solubility vs. 1/T
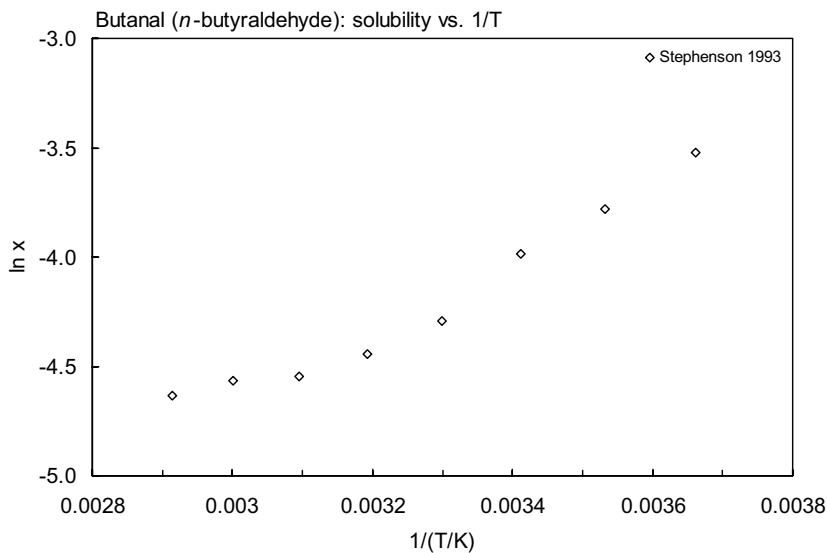
FIGURE 12.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for butanal.

TABLE 12.1.1.4.2
Reported Henry's law constants of butanal (*n*-butyraldehyde) at various temperatures and temperature dependence equations

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

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

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

Zhou & Mopper 1990

gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
fresh water		sea water	
10	3.237	10	4.312
17	-	17	8.660
25	11.65	25	16.08
30	15.83	30	20.68
35	20.68	35	28.15
40	-	40	38.97
45	36.18	45	50.66
eq. 1a	$K_H'/(M/atm)$	eq. 1a	$K_H'/(M/atm)$
A	−8.07	A	−8.20
B	−2704	B	−2698

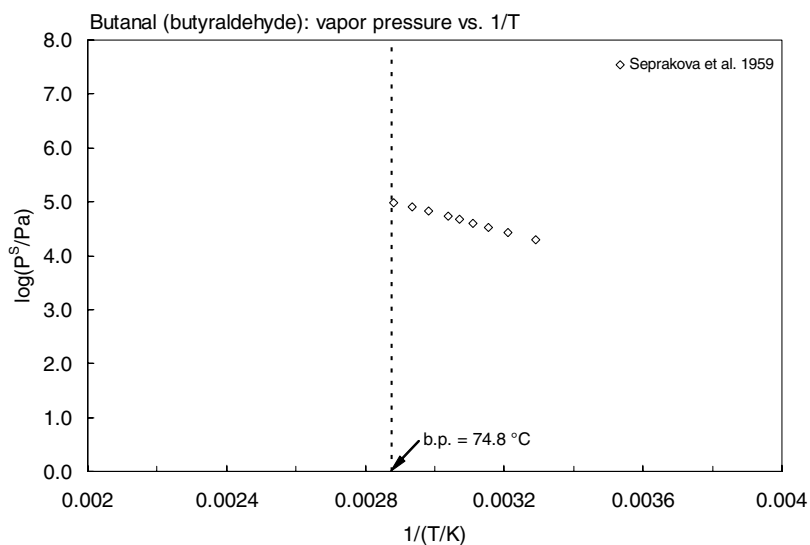**FIGURE 12.1.1.4.2** Logarithm of vapor pressure versus reciprocal temperature for butanal.
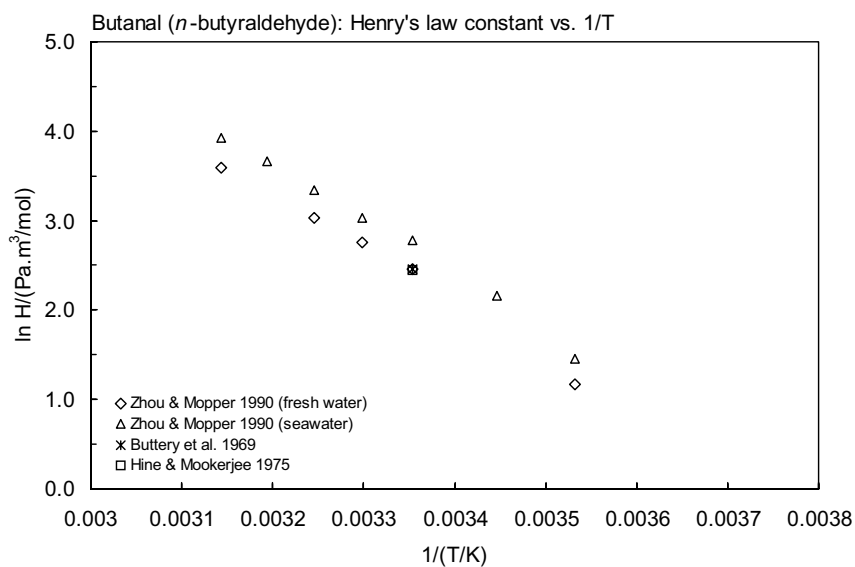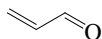

FIGURE 12.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for butanal.

12.1.1.5 2-Propenal (Acrolein)

Common Name: Acrolein
Synonym: 2-propenal, acraldehyde, acrylic aldehyde, allyaldehyde, acrylaldehyde, aqualin
Chemical Name: 2-propenal
CAS Registry No: 107-02-8
Molecular Formula: C_3H_4O, $CH_2=CHCHO$
Molecular Weight: 56.063
Melting Point (°C):
  –87.7   (Lide 2003)
Boiling Point (°C):
  52.6   (Lide 2003)
Density (g/cm³ at 20°C):
  0.8389   (Riddick et al. 1986)
Dissociation Constant:
Molar Volume (cm³/mol):
  66.8   (20°C, calculated-density)
  66.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  208000   (20°C, Günther et al. 1968; Callahan et al. 1979; Verschueren 1977, 1983)
  102020   (shake flask-radioactive analysis, Veith et al. 1980)
  208000   (selected, Riddick et al. 1986)
  229000*, 230000 (20°C, 30°C, shake flask-GC/TC, measured range 0–53°C, Stephenson 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  26664*   (17.5°C, summary of literature data, temp range –64.5 to 52.5°C, Stull 1947)
  log (P/mmHg) = [–0.2185 × 7628.8/(T/K)] + 8.033866; temp range: –64.5 to 52.5°C, (Antoine eq., Weast 1972–73)
  29330, 44000   (20°C, 30°C, Verschueren 1977, 1983)
  35300   (Riddick et al. 1986, Howard 1989)
  36610, 35360   (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
  log (P_L/kPa) = 6.19181 – 1204.95/(–37.8 + T/K); temp range 208–326 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P_L/kPa) = 6.2878 – 1231.003/(–38.405 + T/K); temp range 250–306 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log (P/mmHg) = 57.9815 – 3.0933 × 10³/(T/K) –19.638·log (T/K) + 1.1486 × 10^{-2}·(T/K) – 2.3854 × 10^{-14}·(T/K)²; temp range 185–506 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
  2.84, 13.77 (0, 25°C, headspace-GC, Snider & Dawson 1985)
  12.36   (review, Gaffney et al. 1987)
  0.446   (Howard 1989)
  5.48   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
  log K_{AW} = 4.823 – 2110/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
  –0.09   (quoted, Callahan et al. 1979)
  0.90   (measured value, Veith et al. 1980)

–0.10   (shake flask, Log P Database, Hansch & Leo 1987; recommended, Sangster 1993)
–0.01   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:
   2.54   (bluegill sunfish, Barrows et al. 1980)
   2.54   (bluegill sunfish, Veith et al. 1980)
   –0.22   (estimated-K_{OW}, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
   1.38   (estimated-K_{OW}, Howard et al. 1989)
   –0.219   (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
   Volatilization: $t_{1/2}$ = 10 d from a model river (Howard 1989);
   Photolysis: $t_{1/2}$ = 3.5 d, based on measured quantum yields (Howard 1989).
   Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
      with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
      k_{O3} = 6.4 × 10^{-19} cm^3 molecule^{-1} s^{-1} (Atkinson & Carter 1984)
      k_{OH} = (1.90 – 2.53) × 10^{-11} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in air (Atkinson 1985)
      k_{OH} = 20.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 23.5°C using propylene as reference compound, with a atmospheric
         lifetime of 0.56 d (Edney et al. 1986)
      k_{NO3} = 5.9 × 10^{-16} cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime of 16 d, k_{OH} = 2.0 × 10^{-11} cm^3
         molecule^{-1} s^{-1} with a lifetime of 1.2 d; and k_{O3} = 2.8 × 10^{-19} cm^3 molecule^{-1} s^{-1} with a lifetime of 59 d
         at room temp. (Atkinson et al. 1987)
      k_{OH}(calc) = 2.29 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.96 × 10^{-11} cm^3 molecule^{-1} s^{-1} at room temp. (SAR
         structure-activity relationship, Atkinson 1987)
      k_{OH} = 1.99 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)
      atmospheric $t_{1/2}$ = 3.4–33.7 h, based on rate constant for reaction with OH radical (Howard et al. 1991)
      k_{OH} = 22.9 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 1.15 × 10^{-15} cm^3 molecule^{-1} s^{-1} ((Sabljic & Güsten 1990;
         Müller & Klein 1991)
      k_{OH}(calc) = 17.70 × 10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)
   Hydrolysis: no hydrolyzable groups (Callahan et al. 1979).
   Biodegradation: $t_{1/2}$ = 29 h (natural unsterilized water) and $t_{1/2}$ = 43 h in sterilized (thymol-treated) water (Bowmer &
      Higgins 1976, quoted, Howard 1989);
      aqueous aerobic $t_{1/2}$ = 168–672 h, based on acclimated aqueous screening test data; and aqueous anaerobic
         $t_{1/2}$ = 672–2880 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
   Biotransformation: $t_{1/2}$ < 4 d (Callahan et al. 1979)
   Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:
   Air: atmospheric lifetime of 0.56 d due to reaction with OH radical (Edney et al. 1986);
      calculated atmospheric lifetimes: 16 d for reaction with NO_3 radical, 1.2 d with OH radical and 59 d with
         O_3 (Atkinson et al. 1987);
      $t_{1/2}$ = 10–13 h for reaction with photochemically generated hydroxyl radical, $t_{1/2}$ = 18 d for reaction with
         ozone and $t_{1/2}$ = 3.5 d for photodissociation in the atmosphere (Howard 1989);
      $t_{1/2}$ = 3.4–33.7 h, based on photooxidation half-life in air (Howard et al. 1991);
      atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
   Surface water: removal $t_{1/2}$ = 2.0 to 2.5 d from water (Howard 1989);
   First order k = 0.163 h^{-1} in 8 agricultural canals and varies between 0.104 and 0.211 h^{-1} at pH 7.1 to 7.5 and
      water temperature of 16–24°C, the mean value corresponds to $t_{1/2}$ = 4.25 h at 21°C (Bowmer & Sainty 1977)
      $t_{1/2}$ ~ 8 and 23 d for reacting with singlet oxygen and alkylperoxy radicals in natural sunlit water (estimated,
         Howard 1989),

aqueous aerobic $t_{1/2}$ =168–672 h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2}$ = 672–2880 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

k = 0.015 h^{-1} at 21°C and pH 7.0, corresponding to $t_{1/2}$ = 46 h in dilute buffered solutions of acrolein in distilled water. (Nordone et al. 1996)

Dissipation k = 0.068 h^{-1} with $t_{1/2}$ = 10.2 h and k = 0.028 h^{-1} with $t_{1/2}$ = 7.3 h in weedy (Pump Canal, 12–20°C) and non-weedy agricultural canals (Lateral 1, 12–18°C), respectively, dissipation is the result of numerous processes including degradation, volatilization, adsorption and dilution (Nordone et al. 1996)

Ground water: $t_{1/2}$ = 336–1344 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:

TABLE 12.1.1.5.1
Reported aqueous solubilities and vapor pressures of 2-propenal(acrolein) at various temperatures

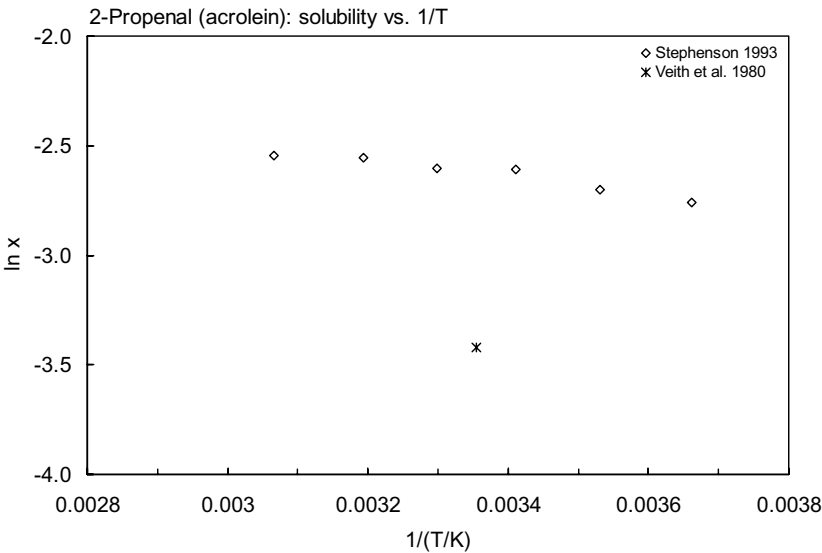| Aqueous solubility		Vapor pressure	
Stephenson 1993		Stull 1947	
shake flask-GC/TC		summary of literature data	
t/°C	S/g·m^{-3}	t/°C	P/Pa
0	197000	−64.5	133.3
10.0	209000	−46.0	666.6
20.0	229000	−36.7	1333
30.0	230000	−26.3	2666
40.0	242000	−15.0	5333
53.0	245000	−7.5	7999
		2.5	13332
		17.5	26664
		34.5	53329
		52.5	101325
		mp/°C	−87.7

FIGURE 12.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-propenal.
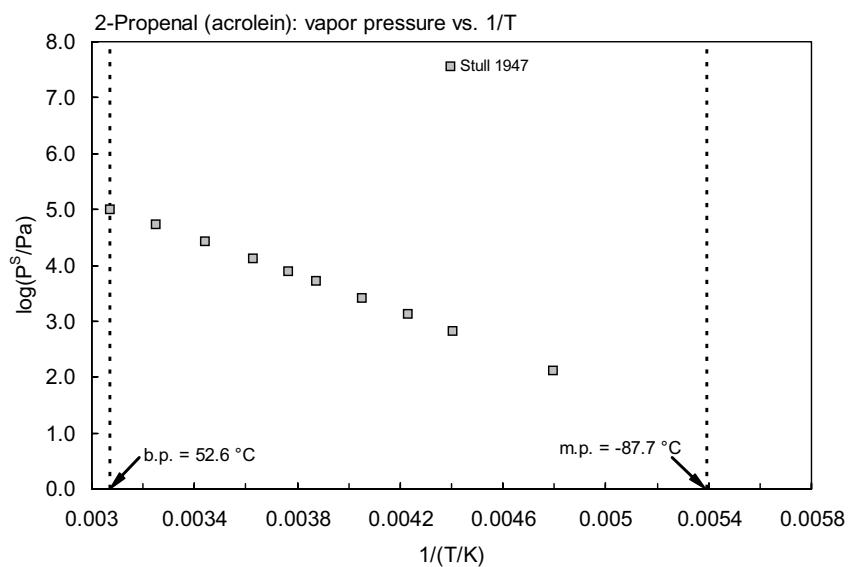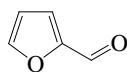
FIGURE 12.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-propenal.

12.1.1.6   Furfural (2-Furaldehyde)

Common Name: Furfural
Synonym: 2-furaldehyde, 2-furancarboxaldehyde; furfurole, 2-furancarbonal, fural, furfuraldehyde, furole
Chemical Name: furfural
CAS Registry No: 98-01-1
Molecular Formula: $C_5H_4O_2$
Molecular Weight: 96.085
Melting Point (°C):
    –38.1   (Lide 2003)
Boiling Point (°C):
    161.7   (Lide 2003)
Density (g/cm^3 at 20°C):
    1.16   (Verschueren 1983)
Dissociation Constant:
Molar Volume (cm^3/mol):
    82.9   (calculated-density, Stephenson & Malanowski 1987)
    92.1   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    82000   (40°C, synthetic method, Jones 1929)
    91593   (shake flask-volumetric method, Booth & Everson 1948)
    92900   (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
    77830   (generator column-HPLC/UV, Tewari et al. 1982)
    79400*, 84000   (20°C, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993)

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

    1066.6*   (39.9°C, ebulliometry, measured range 40–170.6°C, Evans & Aylesworth 1926)
    220.4*   (interpolated-regression of tabulated data, temp range 18.5–161.8°C, Stull 1947)
    1767*   (55.67°C, Ramsay-Young method, measured range 55.6–170°C, Matthews et al. 1950)
    log (P/mmHg) = A – B/(T/K) – C log (T/K); temp range 55.6–170°C (Kirchhoff eq., Matthews et al. 1950)
    log (P/mmHg) = [–0.2185 × 11614.6/(T/K)] + 8.729884; temp range 18.5–161.8°C (Antoine eq., Weast 1972–73)
    133.3, 400   (20°C, 30°C, Verschueren 1983)
    log (P/kPa) = 5.62941 – 1124.583/(148.829 + t/°C), temp rage 92.3–170.6°C (Anotoine eq. derived from Evans & Aylesworth 1926 data, Boublik et al. 1984)
    log (P/kPa) = 5.76606 – 1236.745/(167.368 + t/°C), temp rage 55.87–160.8°C (Anotoine eq. derived from Matthews et al. 1950 data, Boublik et al. 1984)
    208.0   (extrapolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C), temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
    333.3   (Riddick et al. 1986)
    313.2   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P$_L$/kPa) = 6.41784 – 1663.16/(–57.88 + T/K), temp range 357–435 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 32.0337 – 3.3161 × 10^3/(T/K) + 10.171·log (T/K) – 2.1115 × 10^{-2}·(T/K) + 9.2045 × 10^{-6}·(T/K)^2; temp range 237–657 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):
    0.375   (calculated-P/C, Howard 1993)

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

0.34	(20°C, shake flask, Korenman 1972)
0.52	(generator column-HPLC/UV, Tewari et al. 1982)
0.41, 0.52	(shake flask, Log P Database, Hansch & Leo 1987)
0.46	(recommended, Sangster 1993)
0.41	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

0.079	(estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)
–2.097	(estimated-S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

1.602	(soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)
0.00	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1993)

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

Volatilization: based on calculated Henry's law constant, the estimated $t_{1/2} \sim 9.9$ d from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 41.0 mg COD g^{-1} h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

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

Half-Lives in the Environmental Compartments:

Air: estimated photooxidation $t_{1/2} \sim 0.44$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1993).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.6.1
Reported aqueous solubilities of furfural (2-furaldehyde) at various temperatures

Stephenson 1993	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	82200
10.0	78600
20.0	79400
30.0	84000
40.0	89400
50.0	95000
60.0	102800
70.0	109700
80.0	125600
90.0	147400
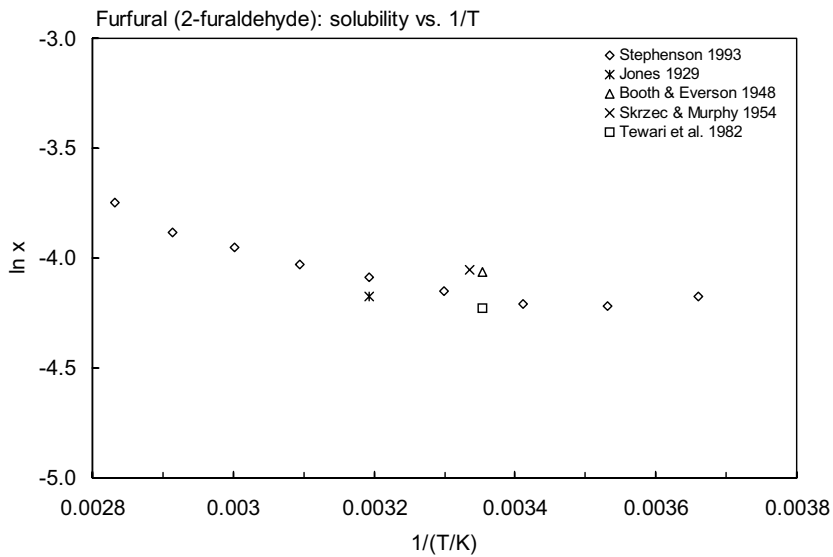
FIGURE 12.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for furfural.

TABLE 12.1.1.6.2
Reported vapor pressures of furfural (2-furaldehyde) at various temperatures and the coefficients for the vapor pressure equations

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

Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						continued	
92.30	9199	18.5	133.3	55.67	1767	139.95	56368
120.3	28531	42.6	666.6	56.07	1793	143.8	61635
131.6	41330	54.8	1333	64.50	2786	146.85	69034
140.2	54795	67.8	2666	67.70	3321	149.65	71727
154.4	83326	82.1	5333	75.05	4600	151.70	77247
159.0	94259	91.5	7999	76.47	5034	153.95	82473
160.9	99192	103.4	13332	84.95	7254	155.10	85459
163.8	108257	121.8	26664	87.38	8239	160.75	101885
170.6	128789	141.8	53329	92.15	9959		
		161.8	101325	93.05	10308	bp/K	433.8
				96.77	12060	$\Delta H_v/(kJ\ mol^{-1}) = 38.59$ at bp	
		mp/°C	−35.6	102.13	15079		
				103.31	15705	Kirchhoff, Rakine, Dupre eq.	
				103.09	17012	eq. 4	P/mmHg
				107.27	18292	A	29.3205
				111.65	21651	B	3530.52
				116.25	24731	C	6.9418
				118.40	27184		
				120.85	29744		
				124.75	34144		

(Continued)

TABLE 12.1.1.6.2 *(Continued)*

Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				126.05	35064		
				126.35	35130		
				132.15	43583		
				133.80	45303		
				135.95	48942		
				138.35	53262		

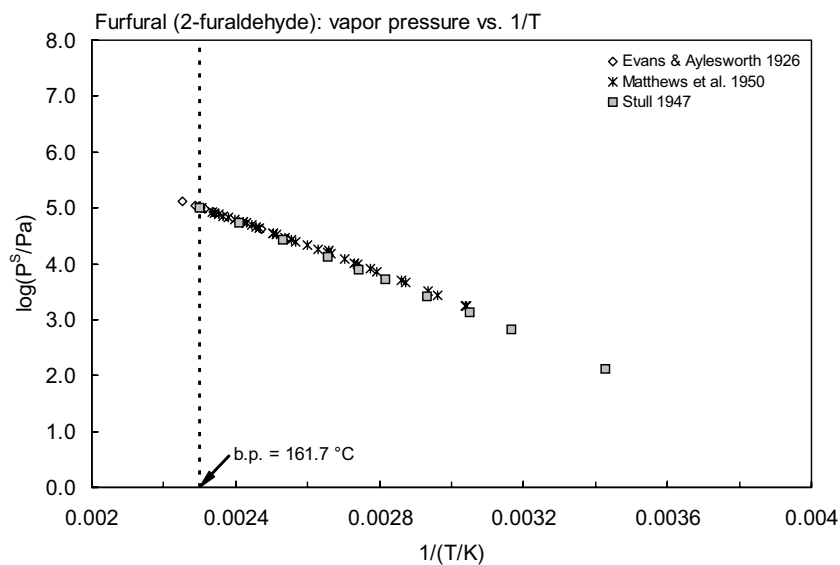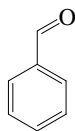**FIGURE 12.1.1.6.2** Logarithm of vapor pressure versus reciprocal temperature for furfural.

12.1.1.7 Benzaldehyde

Common Name: Benzaldehyde
Synonym: benzenecarbonal, oil of bitter almonds
Chemical Name: benzaldehyde
CAS Registry No: 100-52-7
Molecular Formula: C_7H_6O, C_6H_5CHO
Molecular Weight: 106.122
Melting Point (°C):
    –57.1   (Lide 2003)
Boiling Point (°C):
    178.8   (Lide 2003)
Density (g/cm^3 at 20°C):
    1.0401   (24.94°C, measured, Ambrose et al. 1975)
    1.0447   (Dean 1985)
    1.0446   (Riddick et al. 1986)
Molar Volume (cm^3/mol):
    102.0   (calculated-density, Chiou 1985)
    118.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    9.322   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} J/mol K:
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    2991   (quoted, Deno & Berkheimer 1960)
    2857   (1 in 350 parts, Merck Index 1960)
    3490, 3500 (quoted Ph. D. theses from University of London, Mitchell et al. 1964)
    6550, 6580 (shake flask-gravimetric method, shake flask-GC/FID, Mitchell et al. 1964)
    6900–7000 (shake flask-refractive index method, Carless & Swarbrick 1964)
    7200   (20°C, shake flask-GC, Tewari et al. 1982)
    3000   (20–25°C, shake flask-GC, Urano et al. 1982)
    3300   (Verschueren 1983)
    3279   (shake flask-GC, Chiou 1985)
    3000   (20°C, Riddick et al. 1986)
    7200*, 7400 (20°C, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993)
    3514   (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    133.3*, 145.2 (26.2°C, extrapolated-regression of tabulated data, temp range 26.2–179°C, Stull 1947)
    $\log (P/\text{mmHg}) = [-0.2185 \times 11657.8/(T/K)] + 8.580362$; temp range 26.2–179°C (Antoine eq., Weast 1972–73)
    137.0*   (ebulliometry-extrapolated from Antoine eq., measured range 38.5–89.3°C, Ambrose et al. 1975b)
    $\log (P/\text{kPa}) = 6.20251 - 1611.217/(T/K - 67.984)$; temp range 38.5–89.3°C, mercury as reference, Ambrose et al. 1975b
    $\log (P/\text{kPa}) = 6.22556 - 1628.007/(T/K - 66.119)$; temp range 74.9–190.8°C, water as reference, Ambrose et al. 1975b
    169.0   (calculated from different vapor eq., Ambrose et al. 1975)
    160.5   (extrapolated-Antoine eq., Ambrose et al. 1979)
    133.3   (26.0°C, Verschueren 1983)
    160.5   (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.21282 – 1618.669/(205.994 + t/°C); temp range 38.5–208°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

169.0   (Riddick et al. 1986)

log (P_L/kPa) = 5.56823 – 1197.54/(–115.829 + T/K); temp range 348–452 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.4764 – 2455.4/(T/K); temp range 273–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.20256 – 1611.255/(–67.979 + T/K); temp range 409–481 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.48764 – 1782.204/(–52.863 + T/K); temp range 311–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.22745 – 1629.229/(–65.993 + T/K); temp range 370–475 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 28.4711 – 3.4489 × 10^3/(T/K) – 6.8363·log (T/K) – 2.8173 × 10^{-10}·(T/K) + 9.5236 × 10^{-7}·(T/K)^2; temp range 247–695 K (vapor pressure eq., Yaws 1994)

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

2.781, 1.494   (quoted exptl., calculated-bond contribution, Hine & Mookerjee 1975)

2.815   (Gaffney et al. 1987)

2.71*   (gas stripping-GC, measured range 15–45°C, Betterton & Hoffmann 1988)

2.282*   (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –5.00 + 1977/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –5.90 + 2207/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1l), Zhou & Mopper 1990)

3.08*   (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)

ln K_{AW} = –6759/(T/K) + 15.93 (EPICS-UV, temp range 5–25°C, Allen et al. 1998)

1.94   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_{AW} = 4.665 – 2276/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.48   (Leo et al. 1971; Hansch et al. 1972)

1.45   (shake flask-UV at pH 5.62, Umeyama et al. 1971)

1.43   (shake flask-UV, Holmes & Lough 1976)

1.45 ± 0.03   (shake flask at pH 7, Unger et al. 1978)

2.33   (HPLC-RT correlation, Veith et al. 1979)

1.56   (HPLC-k′ correlation, Eadsforth 1986)

1.49   (shake flask, Eadsforth 1986)

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

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

1.48   (recommended, Sangster 1989, 1993)

1.72   (shake flask-UV, Kramer & Henze 1990)

1.48   (shake flask-UV spec., Alcron et al. 1993)

1.48   (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis: loss rate k = 3.4 × 10^{-4} min^{-1} in outdoor Teflon chambers in dark (Grosjean 1985).

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

k < 2.0 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen in the aquatic systems at 25°C with $t_{1/2}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 1.3 \times 10^{-11}$ cm³·molecule⁻¹ s⁻¹ determined by the long-path Fourier transform IR spectroscopic method with reference to that for C_2H_4 or C_2D_4 (Niki et al. 1978)

$k_{OH} = 7.6 \times 10^9$ M⁻¹ s⁻¹ at 25°C with $t_{1/2} = 0.74$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = 7.8 \times 10^{12}$ cm³ mol⁻¹ s⁻¹ at 300 K (Lyman 1982)

$k = (2.5 \pm 0.5)$ M⁻¹ s⁻¹ for 2-10 mM to react with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)

$k_{NO3} = < 9.6 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹ at 300 ± 1 K (using relative rate technique to propene Carter et al. 1981; quoted, Atkinson 1991)

$k_{NO3} = (2.55 \pm 0.08) \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹ at 294 K (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{NO3} = (1.13 \pm 0.25) \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹, compared to a previous measured value $k_{NO3} < 5.2 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate technique, Atkinson et al. 1984)

$k_{OH} = .2 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{NO3} = 2.0 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (reevaluated value, Atkinson et al. 1987)

k_{OH}(exptl) = 1.30×10^{-11} cm³·molecule⁻¹ s⁻¹, k_{OH}(calc) = 1.698×10^{-11} cm³ molecule⁻¹ s⁻¹ (SAR, Atkinson 1987, 1990; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{NO3} = 2.54 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{OH} = 1.29 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 11.40×10^{-12} cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation 119.0 mg COD g⁻¹ h⁻¹ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976),

biodegradation rate constant k = 0.065–0.074 h⁻¹ in 30 mg/L activated sludge after a lag time of 5–10 h (Urano & Kato 1986b).

Biotransformation:

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

Half-Lives in the Environment:

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

$t_{1/2} = 0.74$ d based on rate constants for oxidation by OH radical in the atmosphere at 25°C (Mill 1982);

loss rate k = $(3.4 \pm 1.7) \times 10^{-4}$ min⁻¹ in outdoor Teflon chambers in the dark (Grosjean 1985);

calculated lifetimes of 11 h and 18 d for reactions with OH radical, NO₃ radical, respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.7.1
Reported aqueous solubilities of benzaldehyde at various temperatures

Stephenson 1993	
shake flask-GC/TC	
t/°C	S/g·m⁻³
0	8400
20.0	7200
30.0	7400
40.0	7900
50.0	8200
60.0	9300
70.0	10200
80.0	12400
90.0	14000
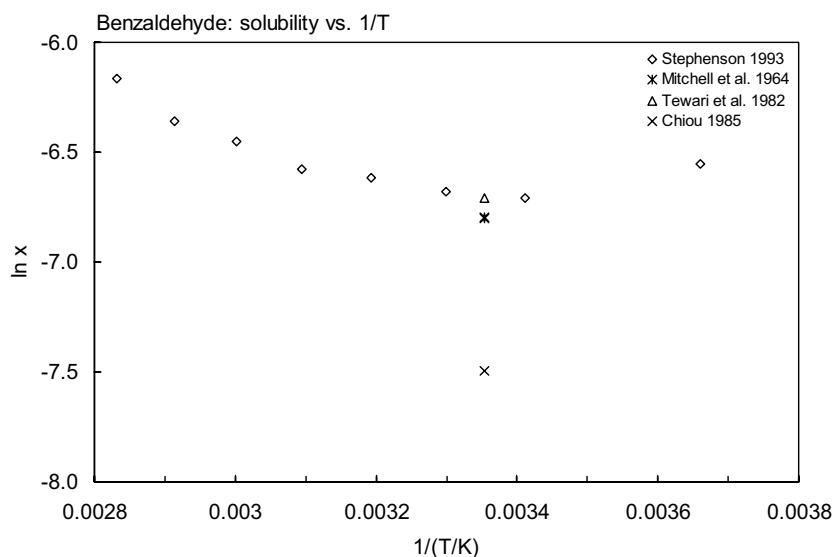
FIGURE 12.1.1.7.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.2
Reported vapor pressures of benzaldehyde at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Ambrose et al. 1975b					
summary of literature data		comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		mercury as reference		water as reference			
26.2	133.3	38.489	399	74.961	2837	25.0	169
50.1	666.6	41.273	473	77.570	3203	31.69	2000
62.0	1333	43.525	539	80.848	3723	76.85	3098
75.0	2666	45.584	608	85.231	4524	178.75	101325
90.1	5333	47.296	672	89.154	5352	213.35	225300
99.6	7999	48.838	722	93.610	6460	254.65	500000
112.5	13332	50.707	814	97.721	7644	421.65	4650000
131.7	26664	51.955	873	102.170	9124		
154.1	53329	56.352	1235	106.662	10854	bp/°C	178.75
179.0	101325	63.266	1592	111.251	12894		
		68.412	2057	115.947	15306	ΔH_V/(kJ mol^{-1}) =	
mp/°C	−26	75.098	2808	120.430	17945	at 25°C	50.3
		77.665	3150	126.350	21995	at bp	42.6
		80.998	3724	131.273	25910		
		83.392	4528	137.178	31339	density	
		89.251	5353	142.836	37379	T/K	ρ/kg m^{-3}
				148.806	44737	292.94	1044.85
				155.366	54140	298.09	1040.13
		Antoine eq.		161.067	63540	298.03	1040.22
		eq. 3	P/kPa	167.121	74923		

TABLE 12.1.1.7.2 *(Continued)*

Stull 1947 summary of literature data		Ambrose et al. 1975 comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		A	6.20251	173.661	88998		
		B	1611.217	178.672	101131		
		C	−67.984	179.710	103800		
				185.556	119891		
				190.829	136055		
				Antoine eq.			
				eq. 3	P/kPa		
				A	6.22556		
				B	1628.007		
				C	−66.119		
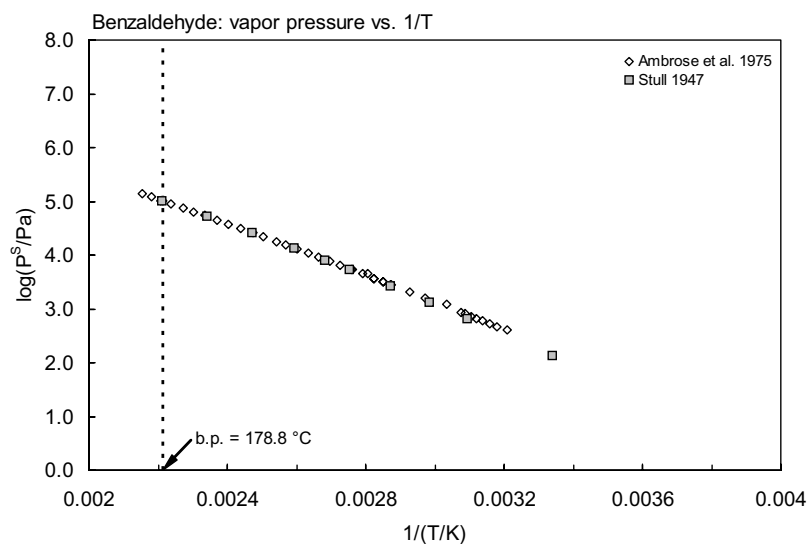
FIGURE 12.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.3

Reported Henry's law constants of benzaldehyde at various temperatures and temperature dependence equations

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

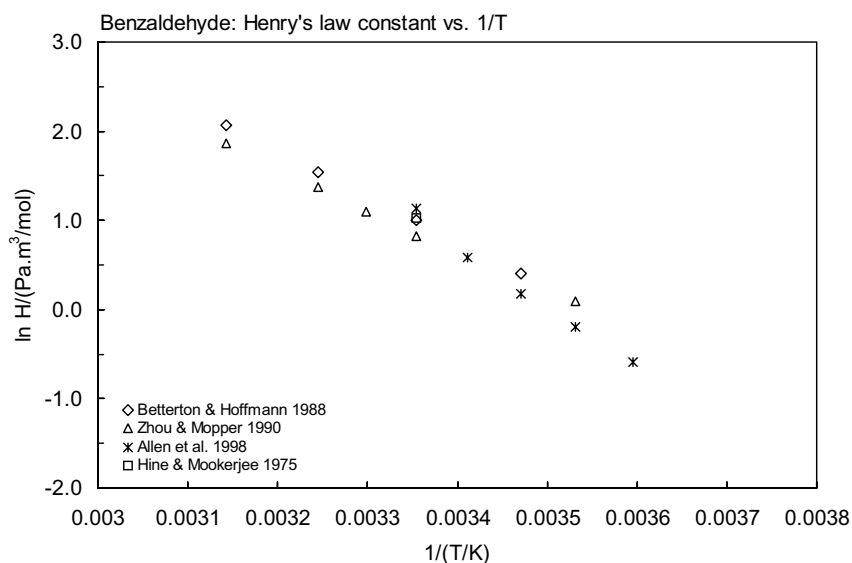| Zhou & Mopper 1990		Zhou & Mopper 1990		Betterton & Hoffmann 1988		Allen et al. 1998	
gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas strpping-GC, spec.		EPICS-UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
	fresh water		sea water				
10	1.095	10	1.339	15	1.506	5	0.555
17	-	17	1.987	25	2.709	10	0.824
25	2.282	25	3.025	35	4.648	15	1.197
30	3.016	30	4.187	45	7.916	20	1.803
35	3.943	35	5.790			25	3.10
40	-	40	7.342				
45	6.413	45	9.296	$\Delta H/(kJ\ mol^{-1}) = -42.2$		eq. 1	K_{AW}
					at 25°C	A	−6759
eq. 1a	$K_H'/(M/atm)$	eq. 1a	$K_H'/(M/atm)$			B	15.93
A	−5.00	A	−5.90				
B	−1977	B	−2207			$\Delta H/(kJ\ mol^{-1}) = -56.2$	
						$\Delta S/(J\ K^{-1}\ mol^{-1}) = 132.4$	

FIGURE 12.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for benzaldehyde.

12.1.2 KETONES

12.1.2.1 Acetone

Common Name: Acetone
Synonym: 2-propanone, dimethylketone, DMK
Chemical Name: acetone, 2-propanone
CAS Registry No: 67-64-1
Molecular Formula: C_3H_6O, CH_3COCH_3
Molecular Weight: 58.079
Melting Point (°C):
    –94.7   (Lide 2003)
Boiling Point (°C):
    56.05   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7899   (Weast 1982–83)
    0.7908   (Dean 1985)
Molar Volume (cm³/mol):
    73.5   (20°C, calculated-density)
    74.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    5.690   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    miscible   (20°C, Palit 1947)
    miscible   (Dean 1985; Yaws et al. 1990)
    miscible   (Riddick et al. 1986; Howard 1990)
    217700, 453000   (pseudo-solubilities, Staples 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    29610*   (interpolated-regression of tabulated data, temp range –59.4 to 56.5°C, Stull 1947)
    log (P/mmHg) = 7.19038 – 1233.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    30490   (Perry 1950)
    51854*   (37.68°C, temp range 37.68–56.02°C, Brown & Smith 1957)
    30800   (Buttery et al. 1969)
    30810   (Hoy 1970)
    29923*   (24.330°C, temp range –12.949 to 55.285°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)
    log (P/mmHg) = [–0.2185 × 10577.7/(T/K)] + 9.143231; temp range –20 to 96°C (Antoine eq., Weast 1972–73)
    30780, 30800 (calculated-Antoine eq., Boublik et al. 1973)
    log (P/mmHg) = 7.15853 – 1231.232/(231.766 + t/°C); temp range 37.6–56.02°C (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1973)
    log (P/mmHg) = 7.11714 – 1210.595/(229.664 + t/°C); temp range –12.95 to 55.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
    30810*   (ebulliometry, fitted to Antoine eq., measured range 259–350.9 K, Ambrose et al. 1974)
    log (P/kPa) = 6.25632 – 1217.904/(T/K – 42.692); temp range 311.7–350.9 K, or for pressure range 53–202 kPa (Antoine eq., ebulliometry, Ambrose et al. 1975a)
    log (P/kPa) = 6.25478 – 1216.689/(T/K – 42.875); temp range 259.17–350.9 K, or for pressure below 225 kPa (Antoine eq., ebulliometry, Ambrose et al. 1974)
    30870, 31520 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.24039 – 1209.746/(229.574 + t/°C); temp range –12.95 to 55.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.26017 – 1214.208/(230.002 + t/°C); temp range –13.98 to 77.72°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)

log (P/kPa) = 6.28185 – 1230.342/(231.665 + t/°C); temp range 37.6–56.02°C (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1984)

30780   (calculated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.11714 – 1210.595/(229.664 + t/°C), temp range: liquid (Antoine eq., Dean 1985, 1992)

24227, 30806 (20, 25°C, Riddick et al. 1986)

log (P/kPa) = 6.25478 – 1216.589/(230.275 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

30730   (interpolated-Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.24204 – 1210.6/(–43.49 + T/K); temp range 261–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.75622 – 1566.69/(0.269 + T/K); temp range 329–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 3.6452 – 469.5/(–108.21 + T/K); temp range 178–243 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.19735 – 1190.382/(–45.373 + T/K); temp range 203–269 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.26483 – 1221.852/(–42.388 + T/K); temp range 257–334 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.24554 – 1211.515/(–43.471 + T/K); temp range 323–379 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.69966 – 1542.465/(0.447 + T/K); temp range 374–464 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

log (P/mmHg) = 28.5884 – 2.469 × 10^3/(T/K) – 7.351·log (T/K) + 2.8025 × 10^{-10}·(T/K) + 2.7361 × 10^{-6}·(T/K)^2; temp range 178–508 K (vapor pressure eq., Yaws 1994)

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

3.34   (partial pressure, Butler & Ramchandani 1935)

3.96   (shake flask, partial vapor pressure-GC, Burnett 1963)

3.25   (28°C, concn. ratio-GC, Nelson & Hoff 1968)

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

4.02, 3.93, 2.91   (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

4.05   (headspace-GC, Vitenberg et al. 1975)

4.10   (calculated-activity coeff and vapor pressure, γ·P, Rathbun & Tai 1982)

0.908, 3.93 (0, 25°C, headspace-GC, Snider & Dawson 1985)

3.38   (review, Gaffney et al. 1987)

2.928*   (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –5.00 + 1977/(T/K); temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

ln [K_H'/(M/atm)] = –3.60 + 1518/(T/K); temp range 25–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1l), Zhou & Mopper 1990)

3.07*   (gas stripping-GC, measured range –14.9 to 44.9°C, Betterton 1991)

4.33   (computed, Yaws et al. 1991)

0.722, 1.26, 2.045, 5.31, 7.514 (0.51, 9.0, 16.11, 31, 38.51°C, headspace-GC, de-ionized water, Benkelberg et al. 1995)

3.735*   (headspace-GC, rain water, measured range –30 to 39.51°C, Benkelberg et al. 1995)

0.762, 2.19, 6.64, 10.30 (0, 14.51, 30, 39.51°C, headspace-GC, artificial seawater, Benkelberg et al. 1995)

ln (k_H/atm) = (18.4 ± 0.3) – (5386 ± 100)/(T/K), temp range 10–40°C (headspace-GC measurements, Benkelberg et al. 1995)

2.56   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

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

2.58   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 3.742 – 1965/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

    –0.24   (shake flask-CR, Collander 1951)
    –0.24   (shake flask at pH 7, Unger et al. 1978)
    –0.48   (shake flask-GC, Tanii et al. 1986)
    –0.24   (recommended, Sangster 1989, 1993)
    –0.31   (CPC centrifugal partition chromatography, Gluck & Martin 1990)
    –0.37   (calculated-UNIFAC activity coeff., Dallos et al. 1993)
    –0.24   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

    –0.187   (calculated, Staples 2000)

Sorption Partition Coefficient, log K_{OC}:

    –0.586   (calculated-K_{OW}, Kollig 1993)
    –0.523   (quoted calculated value, Staples 2000)

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

    Volatilization: using Henry's law constant, $t_{1/2}$ = 20 h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

    Photolysis: rate constant k = 1.4×10^{-5} s^{-1} in the atmosphere (Carlier et al. 1986); calculated lifetime $\tau \sim 60$ d in air (Atkinson 2000)

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

    photooxidation $t_{1/2}$ = 11.3–453 yr, based on measured data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

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

    k_{OH} = $(0.23 \pm 0.03) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 300 K (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

    k_{OH} = $(0.62 \pm 0.09) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (relative rate technique to *n*-hexane, Chiorboli et al. 1983; quoted, Atkinson 1985)

    k = $0.032 \pm 0.006)$ M^{-1} s^{-1} for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

    k_{OH}(calc) = 2.2×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 2.3×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

    photooxidation $t_{1/2}$ = 279–2790 h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

    k_{OH} = 2.16×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 296 K and k = 1.80×10^{-13} cm^3 $molecule^{-1}$ s^{-1} for the aqueous-phase reaction with hydroxyl radical in solution (Wallington & Kurylo 1987)

    k_{OH} = 2.16×10^{-13} cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 1.8×10^{-13} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988)

    k_{OH}* = 2.26×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

    k_{OH}(calc) = 0.18×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1996)

    Hydrolysis:

    Biodegradation: biodegradation rate constants, k = 0.016–0.020 h^{-1} in 30 mg/L activated sludge after a time lag of 20–25 h (Urano & Kato 1986b);

    $t_{1/2}$(aq. aerobic) = 24–168 h, based on unacclimated aqueous screening test data (Bridie et al. 1979; Dore et al. 1975; selected, Howard et al. 1991);

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

k(exptl) = 0.0440 h^{-1} compared to predicted rate constants by group contribution method: k = 0.0433 h^{-1} (nonlinear) and k = 0.043 h^{-1} (linear) (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants:

Half-Lives in the Environment:

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

photooxidation t$_{1/2}$ = 279–2790 h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

calculated lifetimes τ = 53 d and τ > 11 yr for reactions with OH radical, NO$_3$ radical, respectively (Atkinson 2000);

photooxidation and photolysis t$_{1/2}$ = 36 h (Staples 2000).

Surface water: photooxidation t$_{1/2}$ = 11.3–453 yr, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991);

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

aerobic biodegradation t$_{1/2}$ = 96–168 h (Staples 2000).

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

Sediment: anaerobic biodegradation t$_{1/2}$ = 384 h or 16 d (Staples 2000).

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

aerobic biodegradation t$_{1/2}$ = 96–168 h (Staples 2000).

Biota:

TABLE 12.1.2.1.1

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

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

1.

Stull 1947		Brown & Smith 1957		Boublik & Aim 1972			
summary of literature data		Austr. J. Chem. 10, 423-		ref. in Boublik et al. 1984*			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–59.4	133.3	37.68	51854	–12.949	4524	36.649	49704
–40.5	666.6	41.58	60127	–5.424	6967	42.094	61295
–31.1	1333	44.96	68271	–0.103	9306	48.344	77125
–20.8	2666	45.0	68367	4.882	12046	55.285	98572
–9.40	5333	47.01	73603	8.666	14549	bp/°C	56.102
–2.0	7999	49.31	79969	13.019	17921	Antoine eq.	
7.7	13332	51.91	87727	16.831	21314	eq. 2	P/kPa
22.7	26664	56.02	101199	20.939	25780	A	6.24039
39.5	53329			24.330	29923	B	1209.746
56.5	101325			28.351	35493	C	229.574
				32.138	41470		
mp/°C	–94.6						

*ref. Collection Czech. Chem. Commun 37, 3513 (1972)

TABLE 12.1.2.1.1 *(Continued)*

2.

Ambrose et al. 1974

comparative ebulliometry

t/°C	P/Pa	t/°C	P/Pa
		cont'd	
−13.975	4257	55.876	100666
−11.019	5076	56.646	103344
−8.106	6005	60.963	119433
−4.982	7186	64.859	135602
−1.388	8691	69.512	157101
0.288	9497	73.943	180024
1.972	10376	77.724	201571
2.007	10391	25.0	30806
5.493	12417		
5.511	12432	eq. 3	P/kPa
9.077	14840	A	6.25478
9.093	14851	B	1216.689
12.473	17480	C	−42.875
16.928	21525		
20.717	25544		
25.045	30867	**Ambrose et al 1975a**	
29.275	36912		
33.720	44267	bp/°C	56.067
28.601	53675		
42.834	63079	eq. 3	P/kPa
47.320	74449	A	6.25632
52.170	88536	B	1217.904
		C	−42.692

equation for vapor
pressures
below 200 kPa

$\Delta H_V/(\text{kJ mol}^{-1}) =$

at 25°C	31.3
at bp	29.6
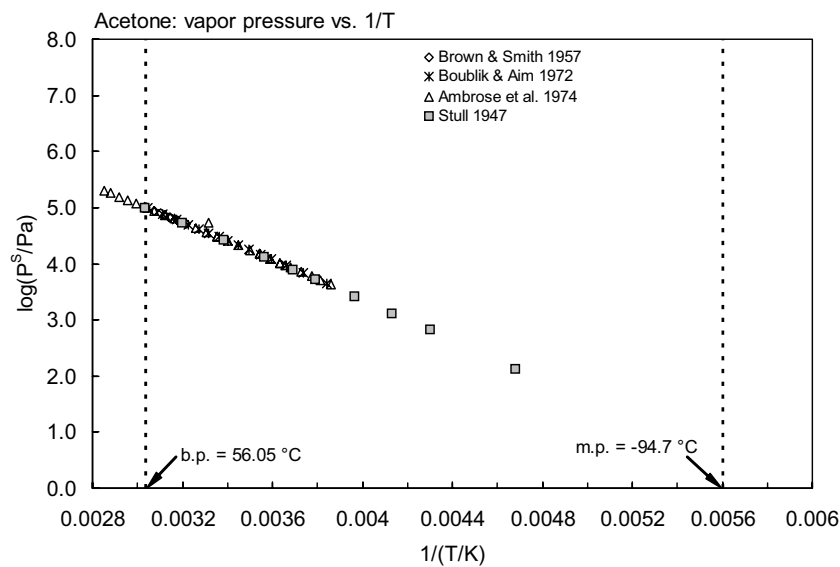
FIGURE 12.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetone.

TABLE 12.1.2.1.2
Reported Henry's law constants of acetone at various temperatures and temperature dependence equations

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

1.

Snider & Dawson 1985		Zhou & Mopper 1990				Betterton 1991	
gas stripping-GC/FID		gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas stripping-GC/FID	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
			fresh water		sea water		
0	0.908	10	1.421	10	1.735	14.9	2.303
25	3.935	17	-	17	2.356	25	3.070
		25	2.846	25	3.311	25	3.269
		30	3.658	30	4.037	25	3.897
enthalpy of transfer		35	4.585	35	4.825	25	3.753
ΔH =	37.24 kJ/mol	40	-	40	5.537	25	3.958
		45	6.178	45	6.846	35.1	7.794
						44.9	11.92
		eq. 1a	K_H'/(M/atm)	eq. 1a	k_H'/(M/atm)		
		A	−5.00	A	−3.60		
		B	−1977	B	−1518		

TABLE 12.1.2.1.2 *(Continued)*

2.

Benkelberg et al. 1995

equilibrium vapor phase concentration-headspace GC

t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
	deionized water		rain water
0.51	0.7222	−28.0	0.742
9.0	1.260	25.0	3.735
16.61	2.0445	39.51	8.328
31.0	5.313		
38.51	7.514		artificial sea water
		0	0.757
for deionized and rain water:		14.51	2.189
eq. 3	k_H/atm	30.0	6.639
A	18.4 ± 0.3	39.51	10.305
B	5286 ± 100		

FIGURE 12.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetone.

12.1.2.2   2-Butanone (Methyl ethyl ketone)

Common Name: Methyl ethyl ketone
Synonym: 2-butanone, butan-2-one, MEK
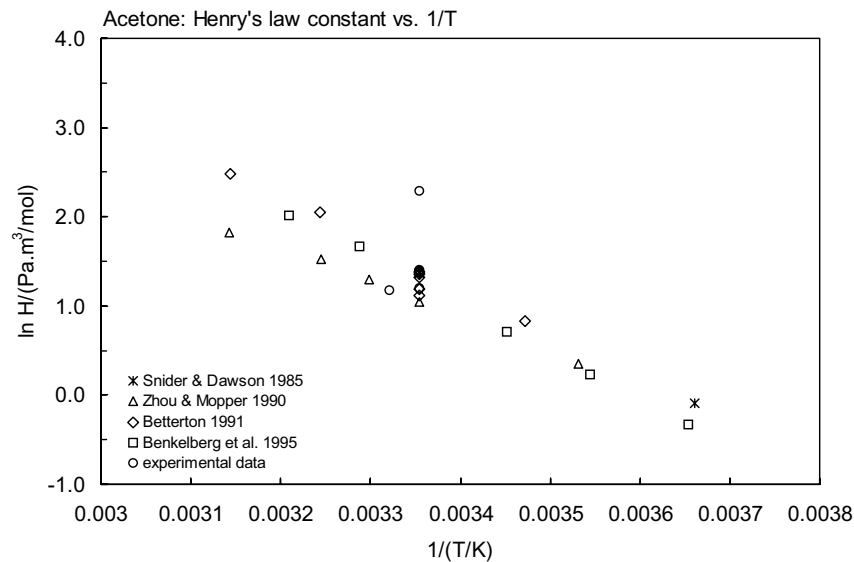Chemical Name: 2-butanone, methyl ethyl ketone
CAS Registry No: 78-93-3
Molecular Formula: C_4H_8O, $CH_3CH_2COCH_3$
Molecular Weight: 72.106
Melting Point (°C):
    –86.64   (Lide 2003)
Boiling Point (°C):
    79.59   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8054   (Weast 1982–83)
    0.7997   (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    89.9   (calculated-density, Rohrschneider 1973)
    96.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    14.7   (pK_a, Riddick et al. 1986)
    –7.2   (pK_{BH}^+, Riddick et al. 1986)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    8.439   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    240000   (20°C, synthetic method, Jones 1929; quoted, Palit 1947; Dean 1985; Riddick et al. 1986)
    255700*   (shake flask-volumetric method, measured range 20–30°C Ginnings et al. 1940)
    343550   (shake flask-volumetric, Ginnings et al. 1940)
    228020   (estimated, McGowan 1954)
    12420   (20°C, Amidon et al. 1975)
    136280   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
    353000   (20°C, Verschueren 1983)
    249000   (selected, Yaws et al. 1990)
    276000*, 235000 (19.3°C, 29.7°C, shake flask-GC, measured range 0–70.2°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
    designated * are compiled at the end of this section):
    12954*   (interpolated-regression of tabulated data, temp range –48.3 to 79.6°C, Stull 1947)
    log (P/mmHg) = 7.22200 – 1343.6/(230 + t/°C), (Antoine eq., Dreisbach & Martin 1949)
    16500*   (31.84°C, ebulliometry, measured range 31.84–79.5°C, Dreisbach & Shrader 1949)
    25158*   (41.46°C, flow calorimetry, measured range 41.46–79.5°C, Nickerson et al. 1961)
    26568*   (42.778°C, ebulliometry, measured range 42.778–88.444°C, Collerson et al. 1965)
    log (P/mmHg) = 7.06376 – 1261.455/(221.982 + t/°C); temp range 42.778–88.444°C (Antoine eq., ebulliometric
        measurements, Collerson et al. 1965)
    log (P/mmHg) = 19.48322 – 2328.0/(T/K) – 3.92657·log (T/K); temp range 42.778–88.444°C (Kirchhoff eq.,
        ebulliometric measurements, Collerson et al. 1965)
    log (P/mmHg) = [–0.2185 × 8149.5/(T/K)] + 7.959295; temp range –48.3 to 79.6°C (Antoine eq., Weast
        1972–73)

12079* (ebulliometry, Ambrose et al. 1975a; quoted, Riddick et al. 1986; Howard 1990)

12000, 12060, 12640 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.02273 – 1167.861/(211.199 + t/°C); temp range 41.46–97.42°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.18397 – 1258.948/(221.725 + t/°C); temp range 42.78–86.44°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

log (P/kPa) = 6.18838 – 1261.297/(222.964 + t/°C); temp range 42.79–88.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

12020 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.06356 – 1261.34/(221.97 + t/°C); temp range 43–88°C (Antoine eq., Dean 1985, 1992)

12700 (Howard et al. 1986; quoted, Banerjee et al. 1990)

12120 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.24715 – 1294.53/(–47.442 + T/K); temp range 294–352 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.18479 – 1259.519/(–51.359 + T/K); temp range 315–363 K (Antoine eq-II., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.22518 – 1286.794/(–47.766 + T/K); temp range 353–403 K (Antoine eq-III., Stephenson & Malanowski 1987)

5425 (calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = 47.706 – 3.0965 × 10^3/(T/K) – 15.184·log (T/K) + 7.4846 × 10^{-3}·(T/K) – 1.7084 × 10^{-13}·$(T/K)^2$; temp range 186–536 K (vapor pressure eq., Yaws 1994)

12071* (static method-manometry, measured range 0–50°C, Garriga et al. 1996)

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

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

4.723 (quoted, exptl., Hine & Mookerjee 1975)

5.549, 4.408 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

3.87 (headspace-GC, Vitenberg et al. 1975)

6.191, 4.215 (calculated-γ·P, calculated-MW, Rathbun & Tai 1982)

0.987, 5.76 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)

13.17* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m³/mol)] = –26.32 – 5214/(T/K), temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)

5.210 (gas stripping-HPLC/UV, Zhou & Mopper 1990)

5.117* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)

ln $[K_H'/(M/atm)]$ = –6.03 + 2184/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

ln $[K_H'/(M/atm)]$ = –5.97 + 2138/(T/K), temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1 l), Zhou & Mopper 1990)

18.28* (45°C, equilibrium headspace-GC, measured range 45–80°C, Ettre et al. 1993)

log $(1/K_{AW})$ = –3.7973482 + 1889.5294/(T/K), temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)

3.85 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

3.95 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 4.764 – 2213/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

5.04 – 3.54 (27°C, equilibrium headspace-GC, solute concn 10.01–85.10 mg/L, measured range 300–315 K, Cheng et al. 2003)

5.04* (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

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

0.26 (shake flask-CR, Collander 1957)

0.28 (shake flask-UV, Fujita et al. 1964, Hansch & Leo 1979)

0.32 ± 0.01 (shake flask-UV, calculated, Iwasa et al. 1965)

0.29 (shake flask-UV, GC, Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1969, 1971)

0.28 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

0.69   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
0.26   (shake flask-GC, Tanii et al. 1986)
0.62   (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.29   (recommended, Sangster 1989, 1993)
0.29   (recommended, Hansch et al. 1995)

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

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

Sorption Partition Coefficient, log K_{OC}:
    1.53   (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)
    1.47 ± 0.55, 1.53 ± 0.88; 1.50 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-
        sorption isotherm, Walton et al. 1992)
    0.070   (predicted-K_{OW}, Walton et al. 1992)
    –0.03   (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
    Volatilization: based on lab. data for evaporation relative to the reaeration rate of 0.27 (Mackay et al. 1982;
        Rathbun & Tai 1982; quoted, Howard 1990) and typical reaeration rates of rivers and lakes (Mill et al. 1982;
        quoted, Howard 1990),
        $t_{1/2}$ = 3 d for evaporation from a river and $t_{1/2}$ = 12 d from lake (Howard 1990).
    Photolysis: rate constant k = 1.4×10^{-5} s^{-1} in the atmosphere (Carlier et al. 1986); calculated lifetime τ ~4 d in
        air (Atkinson 2000)
    Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
        with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression
        see reference:
        photooxidation $t_{1/2}$ = 48.8 – 81.4 yr, based on measured rate data for the reaction with hydroxyl radical in
            aqueous solution (Anbar & Neta 1967; selected, Howard et al. 1991)
        photooxidation $t_{1/2}$ = 2.4 – 24 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of
            disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976)
        k_{OH} = (0.20 ± 0.06) × 10^{10} cm^3 M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)
        k < 2.0×10^2 M^{-1} s^{-1} for oxidation with singlet oxygen at 25°C in aquatic systems with $t_{1/2}$ > 00 yr (Foote
            1976; Mill 1979; quoted, Mill 1982)
        k_{OH} = 1.9×10^9 M^{-1} s^{-1} at 25°C with $t_{1/2}$ = 2.9 d (Hendry & Kenley 1979; quoted, Mill 1982)
        k_{OH} = (0.95 ± 0.09) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at (295 ± 2) K in air (relative rate technique to ethene Cox
            et al. 1981; quoted, Atkinson 1985)
        k_{OH} = (1.20 ± 0.20) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 300 K in air (flash photolysis-resonance fluorescence,
            Zetzsch 1982; quoted, Atkinson 1985)
        k = (0.12 ± 0.02) M^{-1} s^{-1} for the reaction with ozone in water using 20–300 mM t-BuOH as scavenger at
            pH 2 and 20–23°C (Hoigné & Bader 1983)
        k_{OH}(calc) = 1.38×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR
            structure-activity relationship, Atkinson 1985)
        k_{OH} = 0.97×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 24°C with an atmospheric lifetime τ = 12 d (Edney et al. 1986)
        k_{OH} = 1.15×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 296 K and k(soln) = 1.50×10^{-13} cm^3 $molecule^{-1}$ s^{-1} for the aqueous-
            phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)
        k_{OH}* = 1.15×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
        photooxidation $t_{1/2}$ = 64.2 – 642 h, based on measured rate data for the vapor phase reaction with hydroxyl
            radical (Howard et al. 1991)
        k_{OH}(calc) = 1.65×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1996)
    Hydrolysis: first-order hydrolysis $t_{1/2}$ > 0 yr, based on nonreactive hydrolysis from pH 5 to 9 at 15°C (Kollig
        et al. 1987; selected, Howard et al. 1991).

Biodegradation:

$k = 0.021 - 0.025$ h^{-1} in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b)

$t_{1/2}$(aq. aerobic) = 24 – 168 h, based on unacclimated grab sample of aerobic freshwater (Dojilido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

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

$t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(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: $t_{1/2}$ = 2.4–24 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2}$ = 9.8 h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

$t_{1/2}$ = 2.3 d for the atmospheric reaction with photochemically produced hydroxyl radical (Cox et al. 1981; quoted, Howard 1990);

photooxidation $t_{1/2}$ = 64.2–642 h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

calculated atmospheric lifetime τ = 12 d due to reaction with OH radical (Edney et al. 1986) atmospheric transformation lifetime $\tau < 1$ d (estimated, Kelly et al. 1994);

calculated lifetime τ = 10 d for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2}$ = 48.8–81.4 yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2}$ = 24–168 h, based on unacclimated grab sample of aerobic freshwater (Dojlido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

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

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

Sediment:

Soil: calculated $t_{1/2}$ = 4.9 d from first-order kinetic of degradation under both sterile and nonsterile conditions (Anderson et al. 1991);

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

Biota:

TABLE 12.1.2.2.1
Reported aqueous solubilities of 2-butanone (methyl ethyl ketone) at various temperatures

Ginnings et al. 1940		Stephenson 1992	
volumetric method		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	273300	0	367000
25	255700	9.6	310000
30	240700	19.3	276000
		29.7	245000
bp/°C	80.7–80.8	39.6	220000
d^{25}	0.8007	49.7	206000
		60.6	180000
		70.2	182000
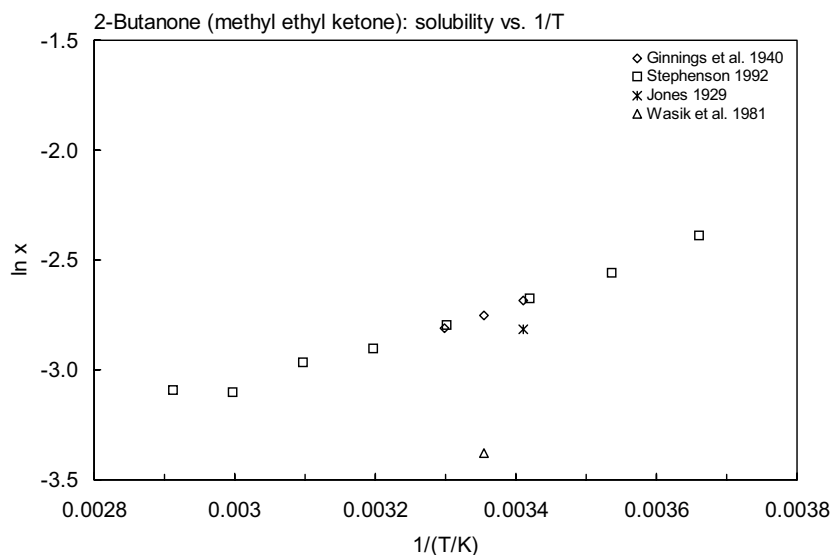
FIGURE 12.1.2.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.2
Reported vapor pressures of 2-butanone (methyl ethyl ketone) at various temperatures and the coefficients for the vapor pressure equations

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

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3) $\ln P = A - B/(C + T/K)$ (3a)

$\log P = A - B/(T/K) - C·\log (T/K)$ (4)

1.

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–48.3	133.3	31.84	16500	41.46	25158	42.778	26568
–28.0	666.6	54.29	42066	65.54	63368	48.148	33024
–17.7	1333	67.36	67661	79.39	101098	53.026	39963
–6.50	2666	79.5	101325	89.43	137282	57.08	46591
6	5333			97.42	173212	60.821	53469
14	7999					64.005	59954
25	13332			eq. 4	P/mm Hg	67.009	66625
41.6	26664			A	21.78963	69.734	73184
60	53329			B	2441.9	72.343	79933
79.6	101325			C	4.70504	74.839	86849
						76.95	93063
mp/°C	–85.9					79.221	100135
						81.268	106887
						83.161	113428
						85.013	120126
						86.715	126547
						88.44	133353
						mp/°C	–86.69
						bp/°C	79.589

TABLE 12.1.2.2.2 *(Continued)*

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						Antoine eq.	
						eq. 2	P/mmHg
						A	7.06376
						B	1261.455
						C	221.982
						Kirchhoff eq.	
						eq. 4	P/mmHg
						A	19.48322
						B	2328
						C	3.92657
						ΔH_V/(kJ mol⁻¹) = 31.67	

2.

Ambrose et al. 1975(a)		Garriga et al. 1996	
comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa
25	12079	5	4277
42.778	26568	10	5644
48.137	33023	15	7334
53.016	39963	20	9435
57.07	46591	25	12071
60.812	53468	30	15281
63.996	59953	35	19110
67.001	66625	40	23682
69.726	73184	45	29132
72.335	79933	50	35540
74.832	86848		
76.944	93063	Antoine eq.	
79.215	100136	eq. 3a	P/kPa
81.262	106887	A	14.133009
83.156	113427	B	2843.871
85.009	120125	C	–53.875
86.711	126545		
88.444	133352		
bp/°C	79.583		
eq. 2	P/kPa		
A	6.18444		
B	1259.223		
C	–51.392		
ΔH_V/(kJ mol⁻¹) =			
at 25°C	34.7		
at bp	31.8		
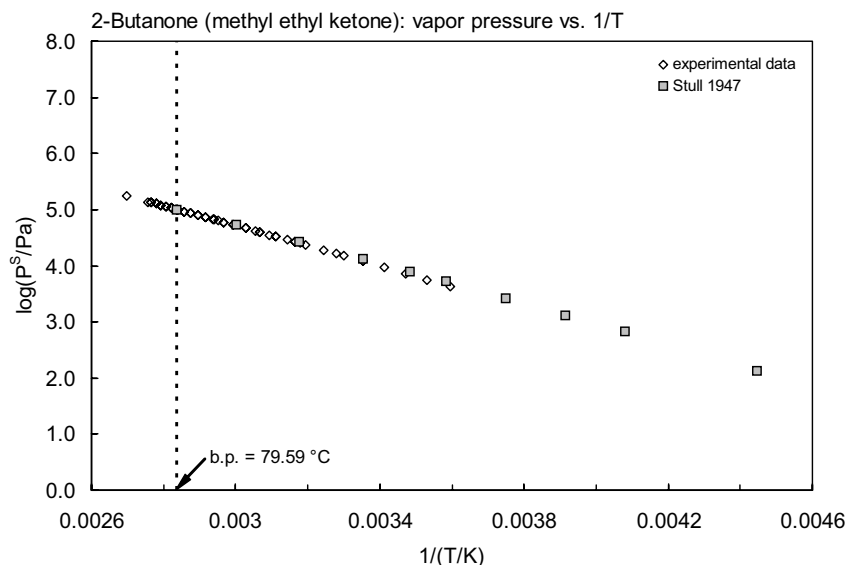
FIGURE 12.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.3
Reported Henry's law constants of 2-butanone (methyl ethyl ketone) at various temperatures and temperature dependence equations

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

Snider & Dawson 1985		Ashworth et al. 1988		Zhou & Mopper 1990			
gas stripping-GC		EPICS-GC		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
					fresh water		sea water
0	0.9873	10	28.37	10	2.068	10	2.702
25	5.765	15	39.52	17	-	17	3.943
		20	19.25	25	5.117	25	6.666
enthalpy of transfer:		25	13.17	30	7.186	30	8.735
ΔH/(kJ mol⁻¹) = 46.024		30	11.15	35	9.296	35	10.78
				40	-	40	14.07
		eq. 4a	H/(atm m³/mol)	45	14.27	45	18.09
		A	−26.32				
		B	−5214	eq. 1a	K$_H'$/(M/atm)	eq. 1a	K$_H'$/(M/atm)
				A	−6.03	A	−5.97
				B	−2184	B	−2138

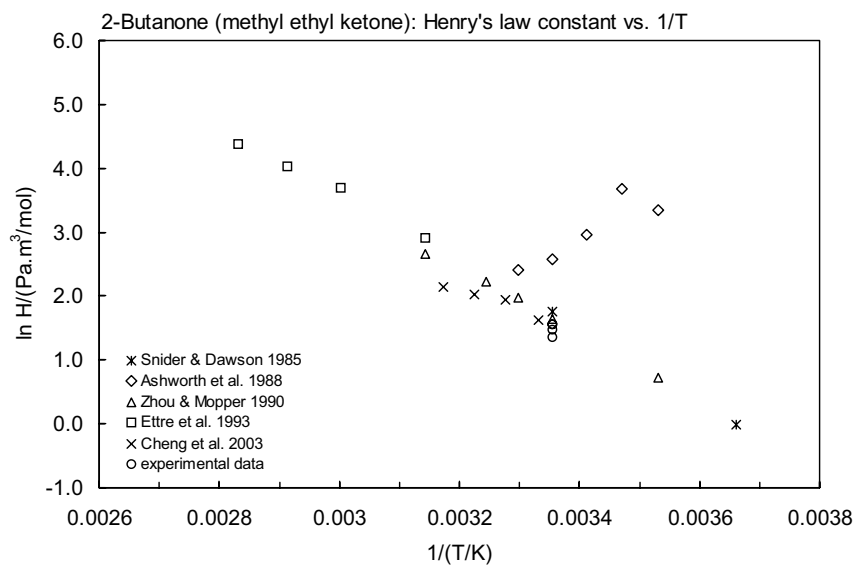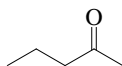**FIGURE 12.1.2.2.3** Logarithm of Henry's law constant versus reciprocal temperature for 2-butanone.

12.1.2.3　2-Pentanone

Common Name: 2-Pentanone
Synonym: 2-pentanone, methyl propyl ketone, methyl *n*-propyl ketone, ethylacetone
Chemical Name: 2-pentanone, methyl propyl ketone
CAS Registry No: 107-87-9
Molecular Formula: $C_5H_{10}O$, $CH_3CH_2CH_2COCH_3$
Molecular Weight: 86.132
Melting Point (°C):
　　–77.80　　　（Stull 1947; Weast 1982–83; Dean 1985; Howard 1990）
　　–76.8　　　（Lide 2003）
Boiling Point (°C):
　　102.0　　　（Weast 1982–83; Verschueren 1983）
　　101.7　　　（Dean 1985; Howard 1990）
　　102.26　　　（Lide 2003）
Density (g/cm³ at 20°C):
　　0.8089　　　　　　（Weast 1982–83）
　　0.8064, 0.8015　　（20°C, 25°C, Riddick et al. 1986）
Molar Volume (cm³/mol):
　　118.4　　　（calculated-Le Bas method at normal boiling point）
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
　　2.541　　　（Riddick et al. 1986）
Entropy of Fusion ΔS_{fus} J/mol K:
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
　　54268*　　（30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939）
　　30150　　（30°C, Gross et al. 1939）
　　55100　　（shake flask-volumetric, Ginnings et al. 1940）
　　59500　　（20°C, shake flask-volumetric, Ginnings et al. 1940）
　　64010　　（shake flask-interferometer, Donahue & Bartell 1952）
　　54350　　（McGowan 1954; Deno & Berkheimer 1960）
　　43000　　（Verschueren 1977, 1983）
　　59500　　（20°C, Riddick et al. 1986）
　　55400　　（selected, Yaws et al. 1990）
　　59000*　　（19.7°C, shake flask-GC, measured range 0–90.5°C, Stephenson 1992）

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
　　2088*　　（interpolated-regression of tabulated data, temp range –12.7 to 102.7°C, Stull 1947）
　　2666　　（28.5°C, Stull 1947）
　　20440*　　（56.649°C, ebulliometry, measured range 56.5–111.655°C, Collerson et al. 1965）
　　log (P/mmHg) = 7.01753 – 1311.145/(214.693 + t/°C); temp range 56.5–111.65°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)
　　log (P/mmHg) = 21.71880 – 2694.12/(T/K) – 4.63307·log (T/K); temp range 56.5–111.65°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)
　　log (P/mmHg) = 6.13916 – 1379.06/(221.41 + t/°C); temp range –5 to 100°C (data fitted to Antoine eq., static method-Ramsey-Young apparatus measurements, Meyer & Wagner 1966)
　　log (P/mmHg) = [–0.2185 × 11240.6/(T/K)] + 9.432089; temp range –12–103.3°C (Antoine eq., Weast 1972–73)
　　4720*　　（ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a）
　　2133　　（quoted, Verschueren 1983）

1621   (quoted, Mackay & Yuen 1983)

4648   (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.14908 - 1311.372/(214.222 + t/°C)$, temp range 61.72–121.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/mmHg) = 7.02193 - 1313.85/(215.01 + t/°C)$, temp range 56–111°C (Antoine eq., Dean 1985, 1992)

4702   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.14243 - 1311.145/(-58.457 + T/K)$, temp range 329–386 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.1404 - 1310.269/(-58.514 + T/K)$, temp range 336–422 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.47975 - 1569.596/(-24.035 + T/K)$, temp range 416–501 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 18.3056 - 2.3477 \times 10^3/(T/K) - 3.6667 \cdot \log (T/K) + 7.1502 \times 10^{-4} \cdot (T/K) + 1.0912 \times 10^{-13} \cdot (T/K)^2$; temp range 196–561 K (vapor pressure eq., Yaws 1994)

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

10.91   (28°C, concn. ratio-GC, Nelson & Hoff 1968)

6.44   (partial vapor pressure-GC, Buttery et al. 1969)

6.52   (quoted, exptl., Hine & Mookerjee 1975)

7.66, 6.52   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

3.83   (calculated-γ·P, Rathbun & Tai 1982)

5.876   (gas-stripping, Hawthorne 1984)

10.13   (modified gas-stripping, Hawthorne et al. 1985)

8.47, 6.83   (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)

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

0.91 ± 0.03 (shake flask-UV at pH 7, Unger et al. 1978)

0.91   (Hansch & Leo 1985)

0.78   (shake flask-GC, Tanii et al. 1986)

0.87   (calculated-V_I and solvatochromic parameters, Kamlet et al. 1988)

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

0.84   (recommended, Sangster 1989; 1993)

0.91   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC}:

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

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

Volatilization: using Henry's law constant, $t_{½}$ = 15.5 h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{½}$ = 14.5 h in a wind-wave tank with a 6m/s wind speed (Howard 1990).

Photolysis:

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

photooxidation $t_{½}$ = 2.4–24 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = (4.64 \pm 0.14) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at (299 ± 2) K (relative rate technique to cyclohexane Atkinson et al. 1982; quoted, Atkinson 1985)

k ~0.02 M^{-1}·s^{-1} for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

k_{OH}(calc) = 4.8×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 4.64×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

k_{OH} = 4.0×10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K and k(soln) = 3.20×10^{-12} cm^3 molecule^{-1} s^{-1} for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

k_{OH} = 4.9×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 5.79×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

k_{OH} = $(4.56 \pm 0.30) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K with calculated tropospheric lifetime τ = 2.5 d (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2}$ = 2.4–24 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2}$ = 3.5 d for reactions with photochemically produced OH radical (Howard 1990);

calculated lifetime τ = 2.5 d for reaction with OH radical (Atkinson 2000).

Surface water: volatilization $t_{1/2}$ = 11–17 h from a model river (Howard 1990).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.3.1
Reported aqueous solubilities of 2-pentanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	76406	20	59500	0	87000
30	54268	25	55100	9.7	69000
50	44362	30	51800	19.7	59000
				31.0	50000
		bp/°C	102.2–102.3	39.6	46000
		d^{25}	0.8018	49.8	42000
				60.1	40000
				70.2	40000
				80.0	38000
				90.5	34000
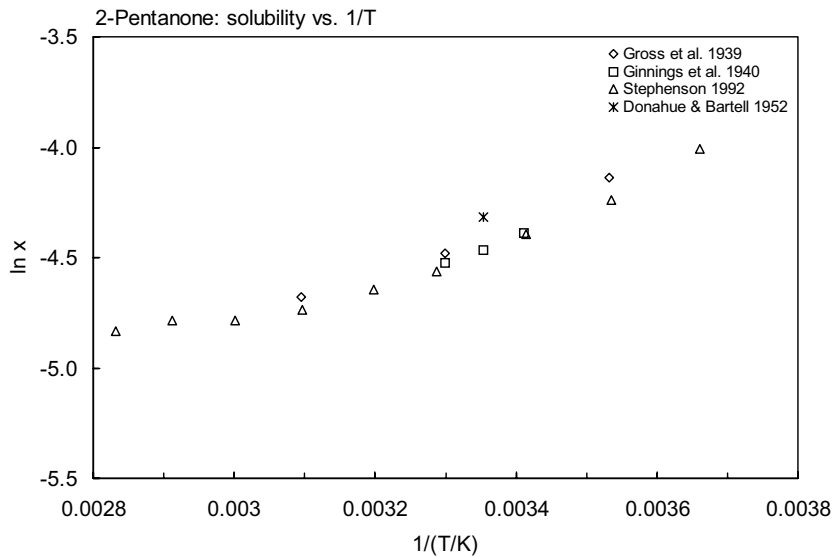
FIGURE 12.1.2.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-pentanone.

TABLE 12.1.2.3.2
Reported vapor pressures of 2-pentanone (methyl propyl ketone) at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−12.0	133.3	56.649	20440	63.175	26546
8	666.6	63.184	26546	68.889	33040
17.9	1333	68.897	33040	74.069	39992
28.5	2666	74.077	39991	78.333	46568
39.8	5333	78.34	46568	82.321	53466
47.3	7999	82.326	53466	85.703	59946
56.8	13332	85.708	59947	88.889	66611
71	26664	88.893	66527	91.832	73283
86.8	53329	91.834	73303	95.547	79906
103.3	101325	94.549	79905	97.178	86760
		97.179	86760	99.47	93107
mp/°C	−77.8	99.47	93107	101.845	100063
		101.345	100062	104.032	106831
		104.031	106831	106.116	113611
		106.114	113612	108.026	120112
		108.023	120113	109.834	126533
		109.83	126535	111.659	133292
		111.655	133283	25	4720
		mp/°C	−76.86	bp/°C	102.262
		bp/°C	102.26		

(Continued)

TABLE 12.1.2.3.2 *(Continued)*

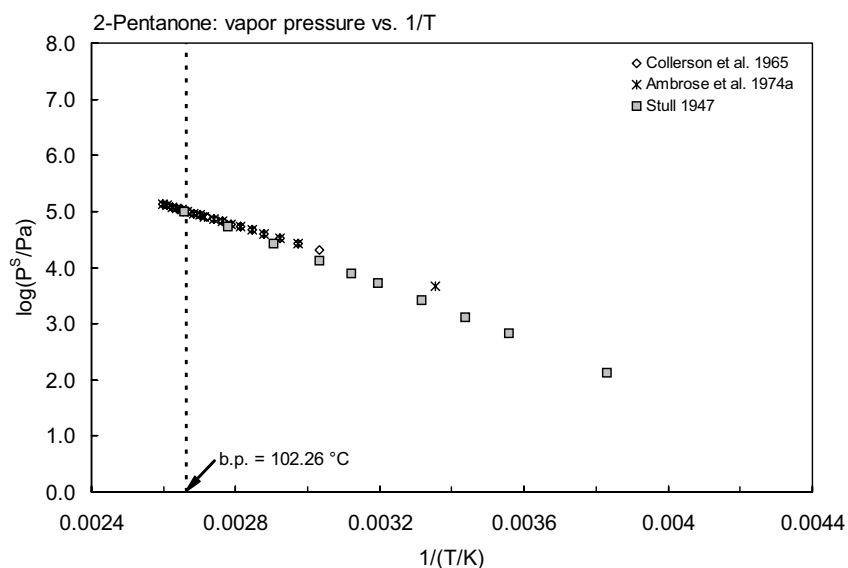| Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		Antoine eq.		eq. 3	P/kPa
		eq. 2	P/mmHg	A	6.13925
		A	7.01753	B	1309.592
		B	1311.145	C	−58.589
		C	214.693		
		Kirchhoff eq		$\Delta H_V/(kJ\ mol^{-1})$ =	
		eq. 4	P/mmHg	at 25°C	38.4
		A	21.7188	at bp	33.6
		B	2594.12		
		C	4.63307		
		$\Delta H_V/(kJ\ mol^{-1})$ = 33.64			

FIGURE 12.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-pentanone.

12.1.2.4   3-Pentanone
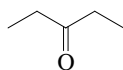
Common Name: 3-Pentanone
Synonym: diethyl ketone, ethylketone, propione, *sym*-dimethylacetone
Chemical Name: 3-pentanone, diethyl ketone
CAS Registry No: 96-22-0
Molecular Formula: $C_5H_{10}O$, $CH_3CH_2COCH_2CH_3$
Molecular Weight: 86.132
Melting Point (°C):
    –39   (Lide 2003)
Boiling Point (°C):
    101.7   (Gross et al. 1933; Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
    0.8138   (Weast 1982–83)
    0.8143, 0.8095   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    92.6   (calculated-density, Jaworska & Schultz 1993)
    118.4   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    27.1   (pK_a, Riddick et al. 1986; Howard 1993)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    11.593   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    46900   (30°C, shake flask-interferometer, Gross et al. 1933)
    49617*   (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)
    49620   (30°C, shake flask-interferometer, Gross et al. 1933)
    48100*   (shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)
    48100   (shake flask-volumetric, Ginnings et al. 1940)
    44520   (shake flask-centrifuge, Booth & Everson 1948)
    43170   (estimated, McGowan 1954)
    47330   (Deno & Berkheimer 1960)
    45650   (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
    47000, 38000 (20°C, 100°C, Verschueren 1983)
    34000   (20°C, Riddick et al. 1986)
    48440   (calculated-fragment solubility const., Wakita et al. 1986)
    53000*   (19.3°C, shake flask-GC, measured range 0–80°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    2169*   (interpolated-regression of tabulated data, temp range –12.0 to 103.3°C, Stull 1947)
    2666   (27.9°C, Stull 1947)
    log (P/mmHg) = 7.25223 – 1450.0/(230 + t/°C), (Antoine eq., Dreisbach & Martin 1949)
    10114*   (36.36°C, ebulliometry, measured range 36.36–101.7°C, Dreisbach & Shrader 1949)
    20441*   (56.649°C, ebulliometry, measured range 56.5–111.3°C, Collerson et al. 1965)
    log (P/mmHg) = 7.027427 – 1309.655/(214.118 + t/°C); temp range 56.5–111.3°C (Antoine eq., ebulliometric
        measurements, Collerson et al. 1965)
    log (P/mmHg) = 22.02258 – 2614.85/(T/K) – 4.72805·log (T/K); temp range 56.5–111.3°C (Kirchhoff eq., ebul-
        liometric measurements, Collerson et al. 1965)

$\log (P/\text{mmHg}) = [-0.2185 \times 11183.0/(T/K)] + 9.406280$; temp range –12.7–102.7°C, (Antoine eq., Weast 1972–73)

4723*   (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

1733   (20°C, Verschueren 1983)

5316, 4714 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.1467 – 1307.941/(213.968 + t/°C)$, temp range 56.53–111.3°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.13703 – 1349.358/(224.351 + t/°C)$, temp range 36.36–101.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4693   (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.02529 – 1310.28/(214.19 + t/°C)$, temp range 56–111°C (Antoine eq., Dean 1985, 1992)

4723   (Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.14917 – 1309.657/(–59.032 + T/K)$, temp range 329–384 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14635 – 1308.327/(–59.137 + T/K)$, temp range 329–426 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.45505 – 1544.596/(–27.379 + T/K)$, temp range 421–502 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

4932   (Daubert & Danner 1989)

$\log (P/\text{mmHg}) = 32.265 – 2.9431 \times 10^3/(T/K) – 8.5068 \cdot \log (T/K) – 4.572 \times 10^{-10} \cdot (T/K) + 2.5177 \times 10^{-6} \cdot (T/K)^2$; temp range 234–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol):

3.617   (calculated-γ·P, Rathbun & Tai 1982)

5.340   (calculated-MW, Rathbun & Tai 1982)

8.834   (calculated-P/C, Howard 1993)

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

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

0.75   (calculated-activity coeff. γ, Wasik et al. 1981)

0.67   (calculated- activity coeff. γ, Berti et al. 1986)

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

0.82   (recommended, Sangster 1989, 1993)

0.99   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.519   (estimated-K_{OW}, Lyman et al. 1990; quoted, Howard 1993)

0.146   (estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

1.914   (soil, estimated-K_{OW}, Lyman et al. 1990; quoted, Howard 1993)

1.08   (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

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

Volatilization: estimated half-life from a model pond of two meter deep is 5.6 d (USEPA 1987; quoted, Howard 1993); based on calculated Henry's law constant, estimated $t_{1/2}$ ~12 h from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

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

photooxidation $t_{1/2}$ = 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.82 \pm 0.33) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 299 ± 2 K in air (relative rate technique to cyclohexane Atkinson et al. 1982)

k_{OH}(calc) $= 2.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) $= 1.82 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

k_{OH}(exptl) $= 2.74 \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} at 296 K; experimentally determined k(soln) $= 2.30 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{OH} = 2.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) $= 3.23 \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to be important (Howard 1993).

Biodegradation: $t_{1/2} \sim 5$ to 10 d in acclimated cultures during screening tests (Howard 1993).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4$–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 5.9$ d, based on an experimentally determined rate constant for the vapor-phase reaction with OH radical in air (Wallington & Kurylo 1987; quoted, Howard 1993).

Surface water: estimated volatilization $t_{1/2} \sim 12$ h in a model river (1 m deep flowing at 1 m/s with a 3 m/s wind) and $t_{1/2} = 5.6$ d in a model environmental pond (2 m deep) (Howard 1993).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.4.1
Reported aqueous solubilities of 3-pentanone at various temperatures

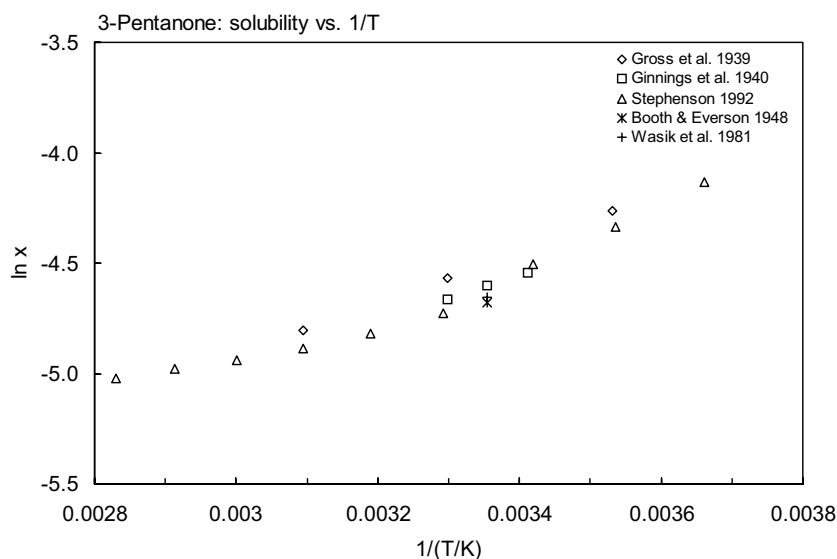| Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	67275	20	50800	0	76800
30	49617	25	48100	9.7	62500
50	39280	30	45000	19.3	53000
				30.6	42400
		bp/°C	101.6–101.9	40.3	38600
		D^{25}	0.8116	50	36200
				60.1	34300
				70.1	33000
				80.2	31500

FIGURE 12.1.2.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 3-pentanone.

TABLE 12.1.2.4.2
Reported vapor pressures of 3-pentanone at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−12.7	133.3	36.36	10114	56.544	20441	56.534	20441
7.5	666.6	51.24	16500	63.032	26530	63.023	26529
17.2	1333	76.04	42066	68.735	33041	68.727	33041
27.9	2666	88.91	67661	73.908	40009	73.901	40009
39.4	5333	101.7	101325	78.158	46590	78.152	46589
46.7	7999			82.114	53473	82.109	53473
56.2	13332			85.494	59947	85.489	59979
70.6	26664			88.612	66532	88.608	66532
86.2	53329			91.605	74147	91.602	73348
102.7	101325			94.314	79985	94.312	79985
				96.897	86752	96.896	86752
mp/°C	−42			99.177	93092	99.176	93093
				101.566	100129	101.567	100129
				103.724	106835	103.725	106834
				105.737	113413	105.739	113412
				107.682	120061	107.685	120059
				109.486	126495	109.489	126493
				111.303	133254	111.307	133252
						25	4723
				mp/°C	−38.97		
				bp/°C	101.959	bp/°C	101.96

TABLE 12.1.2.4.2 *(Continued)*

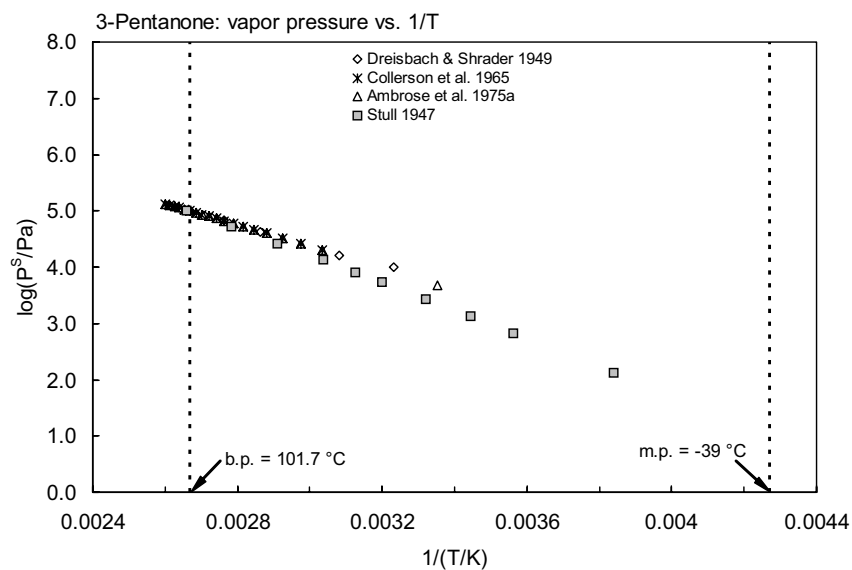| Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Antoine eq		eq. 3	P/kPa
				eq. 2	P/mmHg	A	6.1457
				A	7.02427	B	1307927
				B	1309.653	C	−59.184
				C	214.118		
				Kirchhoff eq. 4, P/mmHg		$\Delta H_V/(kJ\ mol^{-1}) =$	
				A	22.02258	at 25°C	38.6
				B	2614.85	at bp	33.7
				C	4.72085		
				$\Delta H_V/(kJ\ mol^{-1}) = 33.72$			

FIGURE 12.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 3-pentanone.

12.1.2.5   Methyl isobutyl ketone (MIBK)
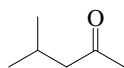
Common Name: Methyl isobutyl ketone
Synonym: hexone, hexanone, 4-methyl-2-pentanone, MIBK
Chemical Name: methyl isobutyl ketone, 4-methyl-2-pentanone
CAS Registry No: 108-10-1
Molecular Formula: $C_6H_{12}O$, $(CH_3)_2CHCH_2COCH_3$
Molecular Weight: 100.158
Melting Point (°C):
    –84   (Lide 2003)
Boiling Point (°C):
    116.5   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7978   (Weast 1982–83)
    0.8010   (Riddick et al. 1986)
Molar Volume (cm³/mol):
    125.0   (20°C, calculated-density)
    140.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    16630*   (30°C, shake flask-interferometer, measured range 0–75°C, Gross et al. 1939)
    19100*   (shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)
    19100   (shake flask-volumetric, Ginnings et al. 1940)
    18200   (shake flask-turbidimeter, McBain & Richards 1946)
    19085   (Deno & Berkheimer 1960)
    17700   (shake flask-radiometric method, Lo et al. 1986)
    17000   (Dean 1985; Riddick et al. 1986)
    19200*   (19.4°C, shake flask-GC/TC, measured range 0–90.4°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    666.6*   (19.7°C, summary of literature data, temp range –1.40 to119°C, Stull 1947)
    2200*   (21.7°C, isoteniscope method, measured range 21.7–116.2°C, Fuge et al. 1952)
    log (P/mmHg) = 31.1616 – 7.7701·log (273.1 + t/°C) – 3173.11/(273.11 + t/°C); temp range 21.7–116.2°C
        (isoteniscope method, Fuge et al. 1952)
    log (P/mmHg) = [–0.2185 × 11669.6/(T/K)] + 9.407655; temp range: –1.4 to119°C, (Antoine eq., Weast
        1972–73)
    800; 1333   (20°C, 30°C, Verschueren 1983)
    2200   (21.7°C, quoted exptl., Boublik et al. 1984; Howard 1990)
    2587   (calculated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.81291 – 1176.833/(192.925 + t/°C), temp range 21.7–116.2°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    2575   (calculated-Antoine eq., Dean 1985)
    log (P/mmHg) = 6.6727 – 1168.4/(191.9 + t/°C), temp range 22–116°C (Antoine eq., Dean 1985, 1992)
    2510   (Riddick et al. 1986)
    log (P/kPa) = 6.0976 – 1190.69/(195.45 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
    2581, 2581 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.79768 – 1168.443/(–81.202 + T/K), temp range 294–390 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.83311 – 1188.115/(–79.265 + T/K), temp range 281–400 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

2687*   (comparative ebulliometry, extrapolated-Antoine eq., measured range 309.7–416 K, Ambrose et al. 1988)

ln (p/kPa) = 14.07841 – 3103.029/(T/K – 61.104); temp range 309.7–416 K (comparative ebulliometry, Ambrose et al. 1988)

log $(P/mmHg)$ = 64.1919 – 4.3577×10^3/(T/K) – 19.766·log (T/K) – 3.9997×10^{-10}·(T/K) + 7.102×10^{-6}·(T/K)^2; temp range 189–571 K (vapor pressure eq., Yaws 1994)

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

39.5*   (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm m^3/mol)] = –7.157 + 160.6/(T/K), temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)

9.523   (calculated-P/C, Howard 1990)

47.95*   (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

ln $(1/K_{AW})$ = –9.56 + 4237/(T/K), temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

45.57   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_{AW} = –1.924 + 57/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.38   (shake flask-GC, Iwasa et al. 1965)
1.09   (calculated-π constant, Hansch et al. 1968)
1.19   (Hansch & Leo, 1979)
1.39   (HPLC-RT correlation, Haky & Young 1984)
1.31   (shake flask-GC, Tanii et al. 1986)
1.38   (recommended, Sangster 1993)
1.31   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

0.301–0.699   (estimated-K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.279–2.025   (soil, estimated-K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)
0.87   (calculated-K_{OW}, Kollig 1993)

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

Volatilization: $t_{1/2}$ = 15–33 h from water of 1 m deep, based on lab. mass-transfer coefficient for volatilization from a stirred 557–2020 rpm water bath at 25°C (Rathbun & Tai 1982; quoted, Howard 1990).

Photolysis: direct photolysis $t_{1/2}$ = 15 h in air (Howard 1990).

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

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

k_{OH} = $(0.9 \pm 0.3) \times 10^{10}$ cm^3 M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

k_{OH}(calc) = 9.4×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 14.1×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2}$ = 4.6–45.5 h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991)

k_{OH} = 14.1×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = (1.31 - 1.45) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (OH radical concn. of 8.0×10^5 molecule·cm^{-3}) at 22–27°C, estimated $t_{1/2} = 16$–17 h (Howard 1990)

k_{OH}(calc) $= 3.92 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to undergo chemical hydrolysis (Howard 1990).

Biodegradation: aqueous aerobic $t_{1/2} = 24$–168 h, based on unacclimated aerobic aqueous screening test data (Bridie et al. 1979; Takemoto et al. 1981; selected, Howard et al. 1991);

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

Biotransformation:

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

Half-Lives in the Environment:

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

photodecomposition $t_{1/2} = 3.5$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

direct photolysis $t_{1/2} = 15$ h and photooxidation $t_{1/2} = 16$–17 h for reactions with hydroxyl radical in air (Howard 1990);

photooxidation $t_{1/2} = 4.6$–45.5 h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

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

Surface water: estimated volatilization $t_{1/2} = 15$–33 h (Howard 1990);

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

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

Sediment:

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

Biota:

TABLE 12.1.2.5.1
Reported aqueous solubilities of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	30749	10	20400	0	29200
10	23137	24	19100	9.5	22100
30	16630	30	17800	19.4	19200
50	14123			30.8	16600
75	13721	bp/°C	115.6–115.7	39.6	14700
		D^{25}	0.7969	50.1	13800
				60.4	12900
				70.2	12400
				80.1	11800
				90.4	12200
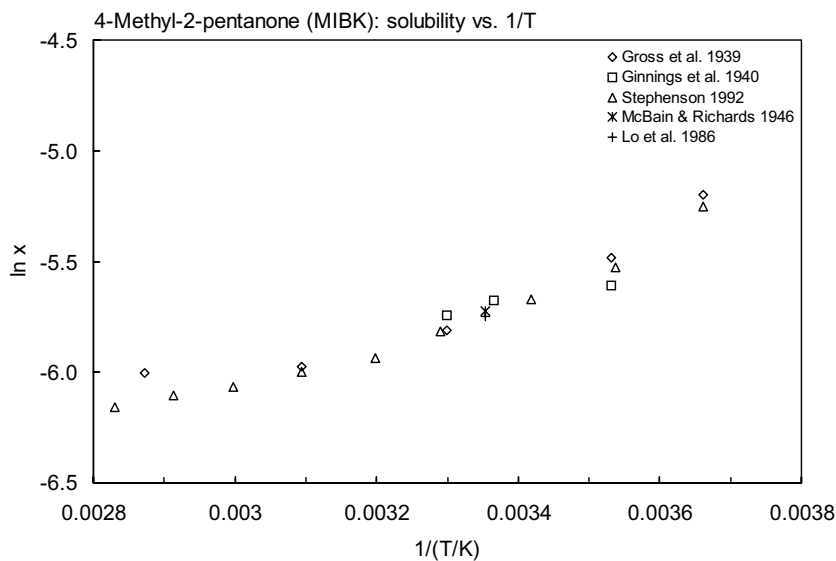
FIGURE 12.1.2.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.2

Reported vapor pressures of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isoteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
−1.40	133.3	21.7	2200	309.676	4922
19.7	666.6	32.7	3933	314.495	6239
30.0	1333	41.4	6266	318.766	7638
40.8	2666	50.2	9266	324.624	9984
52.8	5333	60.0	14999	328.196	11607
60.4	7999	70.0	21598	334.215	15105
70.4	13332	80.1	31997	339.189	18512
85.6	26664	90.9	46396	343.458	21914
102.0	53329	116.2	101325	347.213	25314
119.0	101325			352.107	30381
		bp/K	389.35 K	359.039	38940
mp/°C	−84.7			365.854	49155
		eq. 4	P/mmHg	369.784	55938
		A	31.1616	373.360	62819
		B	3173.11	379.656	76425
		C	−7.7701	383.817	86848
				389.378	101960
				400.202	137928

(Continued)

TABLE 12.1.2.5.2 *(Continued)*

Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
				408.620	172120
				415.823	206364
				298.15	2687
					(extrapolated)
				eq. 3a	P/kPa
				A	14.07841
				B	3103.029
				C	−61.104
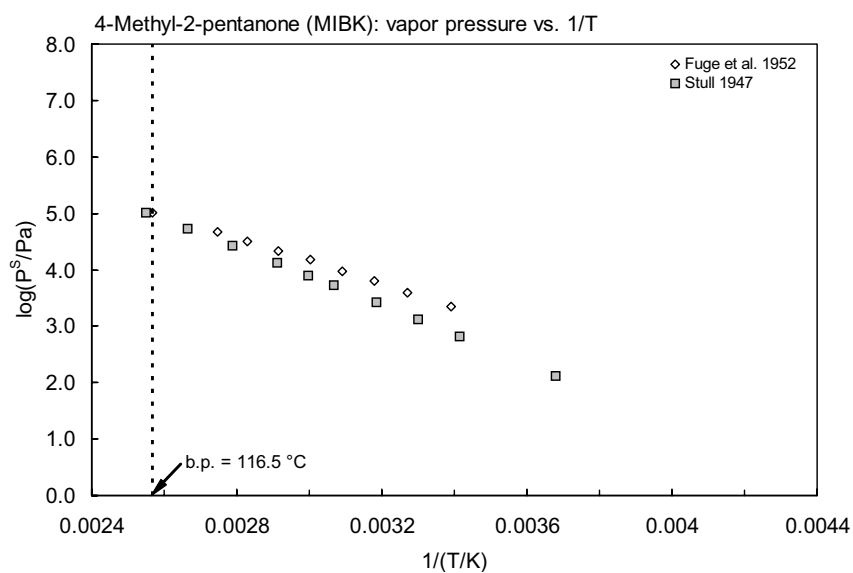
FIGURE 12.1.2.5.2 Logarithm of vapor pressure versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.3
Reported Henry's law constants of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and temperature dependence equations

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

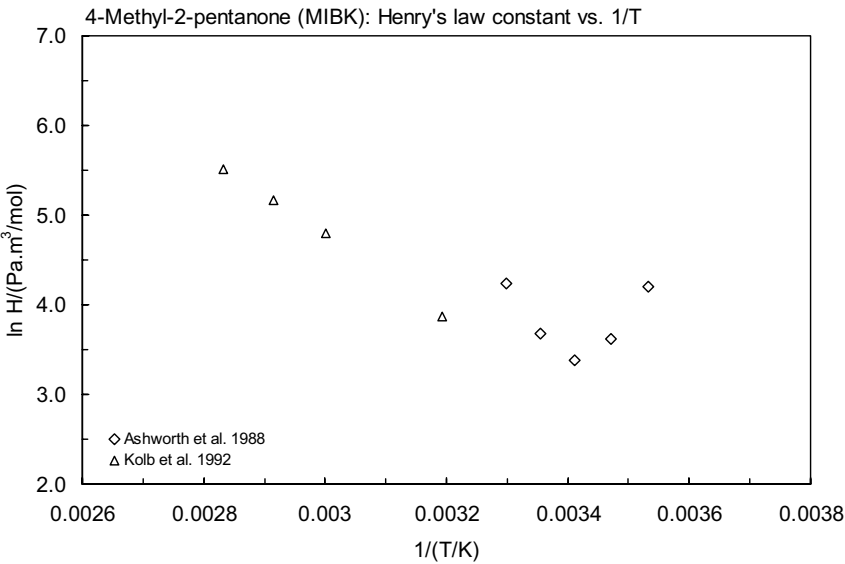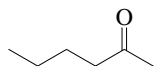| Ashworth et al. 1988		Kolb et al. 1992	
EPICS-GC		**equilibrium headspace-GC**	
t/°C	**H/(Pa m³/mol)**	**t/°C**	**H/(Pa m³/mol)**
10	66.87	40	47.95
15	37.49	60	121.5
20	29.38	70	176
25	39.52	80	248.8
30	68.90		
		eq. 2	$1/K_{AW}$
		A	−9.56
eq. 4a	H/(atm·m³/mol)	B	4237
A	−7.157		
B	160.6		

FIGURE 12.1.2.5.3 Logarithm of Henry's law constant versus reciprocal temperature for 4-methyl-2-pentanone.

12.1.2.6   2-Hexanone (Methyl butyl ketone)

Common Name: Methyl butyl ketone
Synonym: 2-hexanone, methyl *n*-butyl ketone
Chemical Name: 2-hexanone, methylbutyl ketone
CAS Registry No: 591-78-6
Molecular Formula: $C_6H_{12}O$, $CH_3COCH_2CH_2CH_2CH_3$
Molecular Weight: 100.158
Melting Point (°C):
    –55   (Lide 2003)
Boiling Point (°C):
    127.6   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8113   (Weast 1982–83)
    0.8113, 0.8067   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    124.2   (calculated-density, Hoy 1970; Amidon & Williams 1982)
    140.6   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    –8.30   (pK_a, Riddick et al. 1986)
    25.30   (pK_s, Riddick et al. 1986)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    3.56   (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    14523*   (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)
    16400*   (shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)
    16400   (shake flask-volumetric, Ginnings et al. 1940)
    16000   (Erichsen 1952)
    23930   (shake flask-interferometer, Donahue & Bartell 1952)
    15870   (estimated, McGowan 1954)
    16620   (Deno & Berkheimer 1960)
    35000   (20°C, Verschueren 1983)
    17500   (20°C, Riddick et al. 1986)
    15100*, 13700 (19.8°C, 29.7°C, shake flask-GC, measured range 0–91.5°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    514.4*   (interpolated-regression of tabulated data, temp range 7.7–212.6°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 12358.3/(T/K)] + 9.642791; temp range 7.7–127.5°C, (Antoine eq., Weast 1972–73)
    1549*   (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
    509.8   (calculated-Cox eq., Chao et al. 1983)
    266.6   (20°C, Verschueren 1983)
    1540   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.15217 – 1395.406/(208.946 + t/°C), temp range 34.61–154.6°C (Antoine eq. from reported exptl.
        data of Ambrose et al. 1975, Boublik et al. 1984)
    1549   (Riddick et al. 1986)
    log (P/kPa) = 6.16230 – 1401.738/(209.646 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
    1715, 1540 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.4127 - 1575.5/(-43.15 + T/K)$, temp range 293–411 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.14816 - 1392.968/(-64.465 + T/K)$, temp range 279–423 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.15949 - 1399.959/(-63.704 + T/K)$, temp range 310–427 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

1600   (computed-expert system SPARC, Kolling 1995)

log $(P/mmHg) = 4.0508 - 2.6276 \times 10^3/(T/K) + 3.7783 \cdot \log (T/K) - 1.4342 \times 10^{-2} \cdot (T/K) + 8.0592 \times 10^{-6} \cdot (T/K)^2$; temp range 217–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):

9.69   (calculated-P/C, Meylan & Howard 1991)
11.8   (calculated-bond contribution, Meylan & Howard 1991)
9.70   (calculated-P/C, Howard 1993)
8.82   (computed-expert system SPARC, Kolling 1995)

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

1.38   (shake flask-UV, Iwasa et al. 1965; Leo et al. 1971; Hansch & Leo 1979)
1.29   (calculated-π constant, Hansch et al. 1968)
1.39   (HPLC-k′ correlation, Haky & Young 1984)
1.19   (shake flask-GC, Tanii et al. 1986)
1.38   (recommended, Sangster 1989, 1993)
1.38   (recommended, Hansch et al. 1995)
1.30   (computed-expert system SPARC, Kolling 1995)

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

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

Bioconcentration Factor, log BCF:

0.778   (estimated-K_{OW}, Lyman et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

1.322   (soil, estimated-K_{OW}, Lyman et al. 1990)
2.127   (soil, estimated-S, Lyman et al. 1990)
1.10   (computed-K_{OW}, Kolling 1995)

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

Volatilization: $t_{\frac{1}{2}} \sim 135$ h from a model environmental pond of 2 m deep (USEPA 1987; quoted, Howard 1993); using Henry's law constant, $t_{\frac{1}{2}} \sim 12.1$ H from a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

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

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (6.81 \pm 0.29) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at (299 ± 2) K (relative rate technique to cyclohexane, Atkinson et al. 1982; quoted, Atkinson 1985)

k_{OH}(calc) $= 7.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) $= 8.97 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 9.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 9.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 25°C, which corresponds to a half-life of 42 h at an atmospheric OH- concn of 5×10^5 molecule cm^{-3} (quoted, Howard 1993)

k_{OH}(calc) $= 10.57 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: half-life of approximately 5 d in acclimated mixed microbial culture (Howard 1993).

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

Half-Lives in the Environment:

Air: $t_{1/2}$ = 2.4–24 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2}$ ~ 42 h for the vapor-phase reaction with OH radical is 42 h at an atmospheric OH- concentration of 5×10^5 molecule·cm^{-3} (Atkinson 1985; quoted, Howard 1993).

Surface water: volatilization $t_{1/2}$ = 12.1 h from a model river, 135 h from a model environmental pond (Howard 1993).

Ground water:
Sediment:
Soil:
Biota:

TABLE 12.1.2.6.1
Reported aqueous solubilities of 2-hexanone at various temperatures

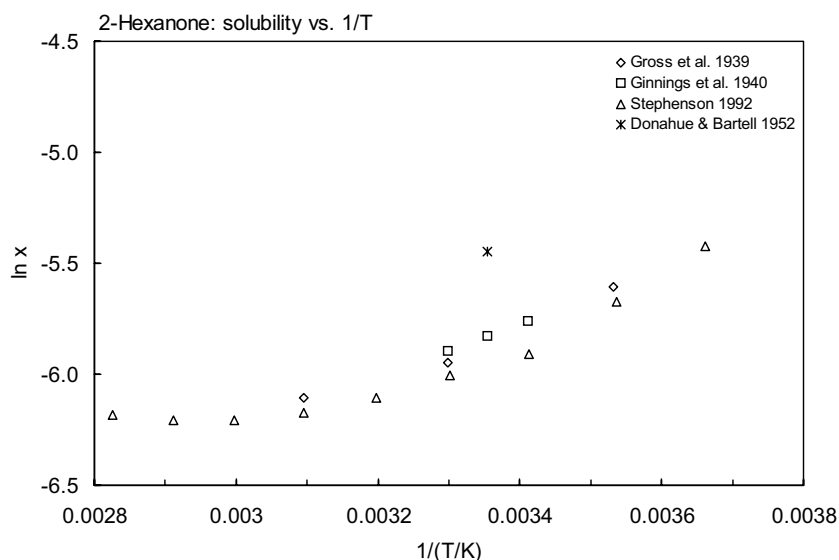| Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
10	20433	20	17500	0	24600
30	14523	25	16400	9.6	19100
50	12420	30	15300	19.8	15100
				29.7	13700
		bp/°C	127.5–127.6	39.6	12400
		d^{25}	0.8072	50.0	11600
				60.5	11200
				70.3	11200
				80.7	11500
				91.5	11900

FIGURE 12.1.2.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-hexanone.

TABLE 12.1.2.6.2
Reported vapor pressures of 2-hexanone at various temperatures and the coefficients for the vapor pressure equations

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

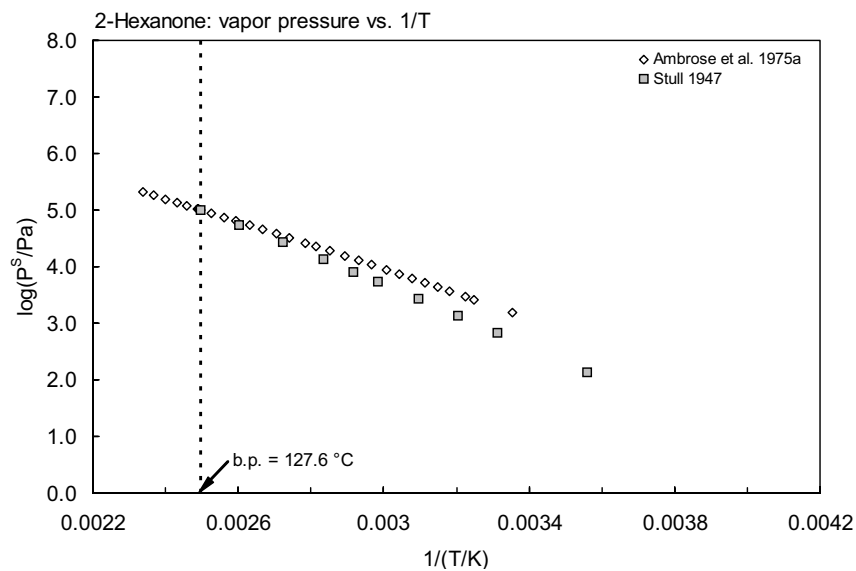| Stull 1947		Ambrose et al. 1975(a)			
summary of literature data		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				cont'd	
7.7	133.3	34.612	2656	128.935	105328
28.8	666.6	37.070	3024	133.789	120447
38.8	1333	41.117	3737	138.034	135072
50.0	2666	44.498	4434	143.528	156043
62.0	5333	48.033	5277	149.390	181140
69.8	7999	51.799	6319	154.613	206034
79.8	13332	55.414	7476	25.0	1549
94.3	26664	59.402	8955		
111.0	53329	63.784	10853	bp/°C	127.583
127.5	101325	67.976	12972		
		72.537	15657	Antoine eq. for full range:	
mp/°C	−56.9	77.315	18944	eq. 3	P/kPa
		82.256	22918	A	6.16230
		86.138	26494	B	1401.738
		91.579	32278	C	−63.504
		96.410	38230	$\Delta H_v/(kJ\ mol^{-1}) =$	
		101.664	45683	at 25°C	42.9
		106.935	54287	at bp	36.0
		112.320	64383		
		117.459	75365	Antoine eq. for restricted range of	
		122.839	88399	of atmospheric pressure:	
		127.231	100312	eq. 3	P/kPa
		127.653	101527	A	6.14801
		128.362	103586	B	1392.870
				C	−64.477

FIGURE 12.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2-hexanone.

12.1.2.7   2-Heptanone
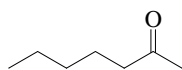
Common Name: 2-Heptanone
Synonym: methyl *n*-amyl ketone, methyl pentyl ketone
Chemical Name: 2-heptanone
CAS Registry No: 110-43-0
Molecular Formula: $C_7H_{14}O$, $CH_3(CH_2)_4COCH_3$
Molecular Weight: 114.185
Melting Point (°C):
    –35   (Lide 2003)
Boiling Point (°C):
    151.05   (Lide 2003)
Density (g/cm³):
    0.81537, 0.81123 (20°C, 25°C, Riddick et al. 1986)
Dissociation Constant:
Molar Volume (cm³/mol):
    141.5   (30°C, Stephenson & Malanowski 1987)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    4300*   (25°C, volumetric method, measured range 20–30°C, Ginnings et al. 1940)
    4054*   (30°C, shake flask-interferometer, measured range 10–75°C, Saylor et al. 1942)
    4546   (estimated, McGowan 1954)
    4300   (Riddick et al. 1986)
    4360*   (19.7°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    521   (interpolated-vapor pressure eq., temp range 4–75°C, Stuckey & Saylor 1940)
    log (P/mmHg) = 7.36537 – 1650.47/(T/K – 54.48); temp range 4–75°C (Antoine eq., Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)
    709*   (30°C, measured range 10–75°C, Saylor et al. 1942)
    133.3*   (19.3°C, summary of literature data, temp range 19.3–150.2°C, Stull 1947)
    log (P/mmHg) = 5.95166 – 1408.13/(194.84 + t/°C); temp range 36 to 151°C (data fitted to Antoine eq., static method-Ramsey-Young apparatus measurements, Meyer & Wagner 1966)
    log (P/mmHg) = [–0.2185 × 12478.9/(T/K)] + 9.305642, temp range 19.3–150.2°C, (Antoine eq., Weast 1972–73)
    427*   (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
    log (P/mmHg) = [1– 400.348/(T/K)] × 10^{0.934881 – 4.87941 × 10^{-4}·(T/K) + 4.16258 × 10^{-7}·(T/K)²}; temp range 280.85–400.65 K, (Cox eq., Chao et al. 1983)
    514   (Abraham 1984; Riddick et al. 1986)
    504   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.14611 – 1460.276/(201.636 + t/°C), temp range 94.7–179.3°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
    469   (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.07656 – 1408.73/(–78.31 + T/K), temp range 303–424 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15178 - 1464.092/(-71.076 + T/K)$, temp range 327–457 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.56718 - 1810.283/(-26.944 + T/K)$, temp range 449–580 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -13.0256 - 2.6425 \times 10^3/(T/K) + 11.879 \cdot \log (T/K) - 2.7571 \times 10^{-2} \cdot (T/K) + 1.456 \times 10^{-5} \cdot (T/K)^2$; temp range 238–612 K (vapor pressure eq., Yaws 1994)

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

14.63	(partial vapor pressure-GC, Buttery et al. 1969)
14.6; 14.94, 14.6	(exptl.; calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
5.715	(calculated-activity coefficient γ·P, Rathbun & Tai 1982)
9.120	(calculated-P/C, Mackay & Yuen 1983)
16.0	(correlated-molecular structure, Russell et al. 1992)
17.1	(gas stripping-GC, Shiu & Mackay 1997)

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

2.08	(calculated-activity coefficients, Wasik et al. 1981)
1.98	(generator column-HPLC, Tewari et al. 1982)
2.00	(shake flask-GC, Tanii et al. 1986)
2.03	(calculated-UNIFAC activity coefficients, Dallos et al. 1993)
1.98	(recommended, Sangster 1993)
1.98	(recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{OH} = (8.67 \pm 8.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 296 K (Wallington et al. 1987; quoted, Atkinson 1989)

k_{OH}(calc) = 13.10×10^{-12} cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

$k_{OH} = (1.17 \pm 0.11) \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K with calculated tropospheric lifetime τ = 1.0 d (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetime τ = 1.0 d, based on gas-phase reaction with OH radical (relative rate method, Atkinson et al. 2000)

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.7.1
Reported aqueous solubilities of 2-heptanone at various temperatures

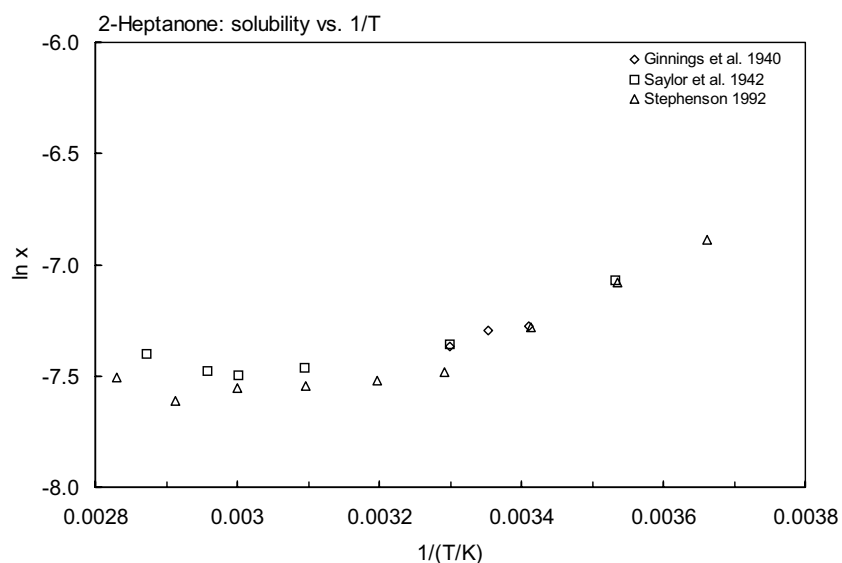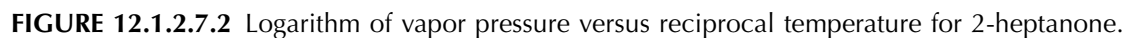| Ginnings et al. 1940		Saylor et al. 1942		Stephenson 1992	
volumetric method		shake flask-interferometer		shake flask-GC/TC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
20	4400	10	5390	0	6490
25	4300	30	4054	9.7	5350
30	4000	50	3643	19.8	4360
		60	3517	30.7	3580
bp/°C	151.2–151.3	65	3597	39.7	3430
d²⁵	0.8115	75	3871	49.8	3360
				60.2	3330
				70.1	3140
				80.2	3480
				90.5	3530

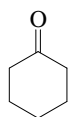**FIGURE 12.1.2.7.1** Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-heptanone.

TABLE 12.1.2.7.2
Reported vapor pressures of 2-heptanone at various temperatures and the coefficients for the vapor pressure equations

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

Stuckey & Saylor 1940		Stull 1947		Ambrose et al. 1975(a)			
static method-Hg manometer		summary of literature data		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						cont'd	
data presented as		19.3	133.3	54.687	2818	151.949	103789
eq. 3	P/mmHg	43.5	666.6	57.076	3180	157.300	119605
A	7.36537	55.5	1333	60.142	3697	162.280	136005
B	1650.47	67.7	2666	64.213	4500	168.137	157388
C	−54.48	81.2	5333	67.814	5324	173.697	180116
		89.8	7999	71.989	6433	179.267	205316
		100.0	13332	71.991	6436	25.0	427
		116.1	26664	75.736	7617		
Saylor et al. 1942		133.2	53329	79.945	9127	bp/°C	151.058
Stuckey & Saylor data		150.2	101325	84.035	10826		
10	188			88.302	12873	Antoine eq. for full range:	
30	709	mp/°C	–	92.564	15282	eq. 3	P/kPa
50	1973			95.832	17932	A	6.15034
60	3733			102.322	21975	B	1462.981
65	4720			107.012	25997	C	−71.24
75	7413			112.377	31321	$\Delta H_V/(kJ\ mol^{-1}) =$	
				117.486	37167	at 25°C	38.3
				117.629	37361	at bp	33.2
				123.186	44713		
				129.297	54129	Antoine eq. for restricted	
				134.589	63526	range of atm. pressure:	
				140.221	74904	eq. 3	P/kPa
				146.323	88989	A	6.15033
				150.976	101114	B	1463.072
						C	−71.200

FIGURE 12.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for 2-heptanone.

12.1.2.8   Cyclohexanone

Common Name: Cyclohexanone
Synonym:
Chemical Name: cyclohexanone
CAS Registry No: 108-94-1
Molecular Formula: $C_6H_{10}O$
Molecular Weight: 98.142
Melting Point (°C):
    –27.9   (Lide 2003)
Boiling Point (°C):
    155.43   (Lide 2003)
Density (g/cm³ at 20°C):
    0.9478   (Weast 1982–83; Dean 1985)
    0.9452   (Riddick et al. 1986)
Molar Volume (cm³/mol):
    106.2   (calculated-density, Stephenson & Malanowski 1987)
    118.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    23000   (Riddick et al. 1986)
    93200   (selected, Yaws et al. 1990)
    97000*, 82000   (19.5°C, 29.8°C, shake flask-GC, measured range 0–90.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
    designated * are compiled at the end of this section):
    666.6*   (26.4°C, summary of literature data, temp range 1.4–155.6°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 10037.6/(T/K)] + 8.019908; temp range 1.4–155.6°C, (Antoine eq., Weast 1972–73)
    533*   (ebulliometry-fitted to Antoine eq., temp range 89.6–165.8°C, Meyer & Hotz 1973)
    log (P/mmHg) = 5.978401 – 1495.511/(209.5517 + t/°C); temp range 89.6–165.8°C (Antoine eq. ebulliometric
        measurements, Meyer & Hotz 1973)
    614   (interpolated-Cox eq., Chao et al. 1983)
    log (P/mmHg) = [1– 428.587/(T/K)] × 10^{0.833332 – 6.42578 × 10⁻⁴·(T/K) + 7.09855 × 10⁻⁷·(T/K)²}; temp
        range: 274.55–438.92 K (Cox eq., Chao et al. 1983)
    533   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.10133 – 1494.166/(209.399 + t/°C), temp range 89.29–165.8°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    640   (Riddick et al. 1986)
    log (P/kPa) = 6.103304 – 1495.511/(209.5517 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
    620, 534 (calculated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P_S/kPa) = 8.434 – 2576.6/(T/K); temp range not specified (Antoine eq., solid, Stephenson & Malanowski
        1987)
    log (P_L/kPa) = 6.103304 – 1495.511/(–63.5983 + T/K), temp range 362–439 K (Antoine eq.-II, liquid,
        Stephenson & Malanowski 1987)
    log (P/mmHg) = 70.5022 – 4.412 × 10³/(T/K) – 23.605·log (T/K) + 1.1205 × 10⁻²·(T/K) – 1.5648 × 10⁻¹³·(T/K)²;
        temp range 242–629 K (vapor pressure eq., Yaws 1994)

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

    1.216   (Hawthorne et al. 1985)
    2.266   (calculated-P/C, Meylan & Howard 1991)
    5.179   (estimated-bond contribution, Meylan & Howard 1991)

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

    0.81   (shake flask, Hansch & Leo 1979, 1985, 1987)
    0.81   (recommended, Sangster 1989, 1993)
    0.81   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

    0.39   (calculated-K_{OW} with regression eq., Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

    1.00   (calculated-S, K_{OW} with regression eq., Roy & Griffin 1985; quoted, Howard 1990)

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

    Volatilization: using Henry's law constant, $t_{1/2} \sim 3.1$ d from a model river 1-m deep flowing 1 m s^{-1} with wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1990).

    Photolysis: direct sunlight photolysis rate constant of about 0.16 d^{-1} corresponding to $t_{1/2} = 4.3$ d (Mill & Davenport 1986; quoted, Howard 1990).

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

        photooxidation $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

        $k_{OH} = 1.56 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 25°C with $t_{1/2} \sim 1$ d (Atkinson 1985; quoted, Howard 1990)

        $k_{OH} = 6.39 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at 298 K (Atkinson 1989)

        $k_{OH} = 12.55 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} from Atmospheric Oxidation Program, k_{OH}(exptl) $= 6.39 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} and k_{OH}(calc) $= 2.92 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

        k_{OH}(calc) $= 5.09 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

    Hydrolysis:

    Biodegradation: average rate of biodegradation 51.5 mg COD g^{-1} h^{-1} based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

    Biotransformation:

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

Half-Lives in the Environment:

    Air: $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);

        degrade rapidly by reaction with sunlight produced hydroxyl radicals with $t_{1/2} \sim 1$ d and by direct sunlight photolysis with $t_{1/2} \sim 4.3$ d (Howard 1990).

    Surface water: estimated $t_{1/2} \sim 0.003$ yr at Noordwijk (Zoeteman et al. 1981).

    Ground water:

    Sediment:

    Soil:

    Biota:

TABLE 12.1.2.8.1
Reported vapor aqueous solubilities and vapor pressures of cyclohexanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log (P/atm) = A'[1 - (T_B/T)]$	(5)	where $A' = (a + bT + cT^2)$	

Aqueous solubility		Vapor pressure			
Stephenson 1992		Stull 1947		Meyer & Hotz 1973	
shake flask-GC/TC		summary of literature data		comparative ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
0	137000	1.40	133.3	89.628	12725
9.8	115000	26.4	666.6	94.986	15528
19.5	97000	38.7	1333	100.807	19257
29.8	82000	52.5	2666	107.664	24477
40.1	75000	67.8	5333	114.303	30580
50.2	70000	77.5	7999	119.712	36416
60.5	67000	90.4	13332	125.282	43337
71.1	65000	110.3	26664	130.659	50990
80.2	68000	132.5	53329	135.774	59239
90.7	69000	155.6	101325	141.742	70181
				145.880	78656
		mp/°C	–45.0	151.916	92474
				151.969	92593
				156.917	105300
				156.988	105417
				165.769	131422
				bp/°C	155.422
				Antoine eq.	
				eq. 2	P/cmHg
				A	5.978401
				B	1495.511
				C	209.5517
				Cox eq.	
				eq. 5	P/atm
				a	0.852046
				$-b \times 10^3$	0.612660
				$c \times 10^6$	0.504661
				T_B/K	428.5716
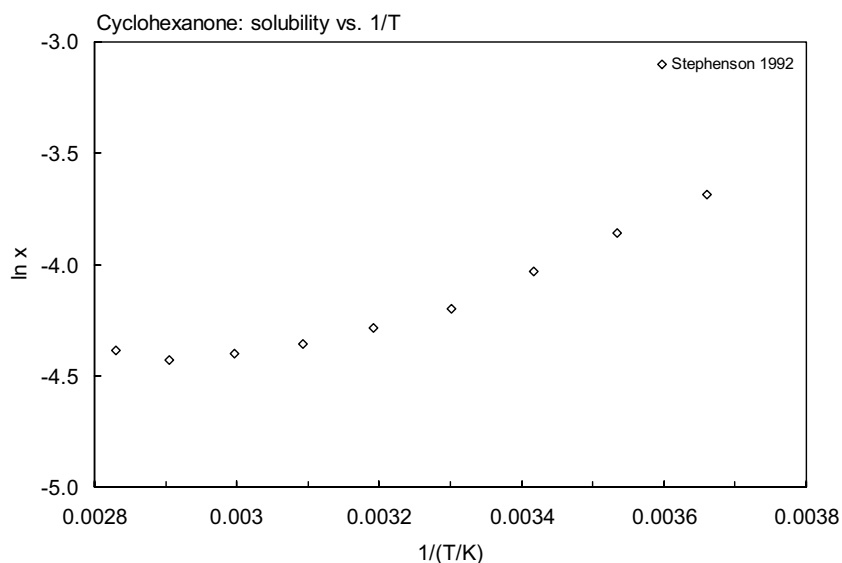
FIGURE 12.1.2.8.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for cyclohexanone.

FIGURE 12.1.2.8.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanone.
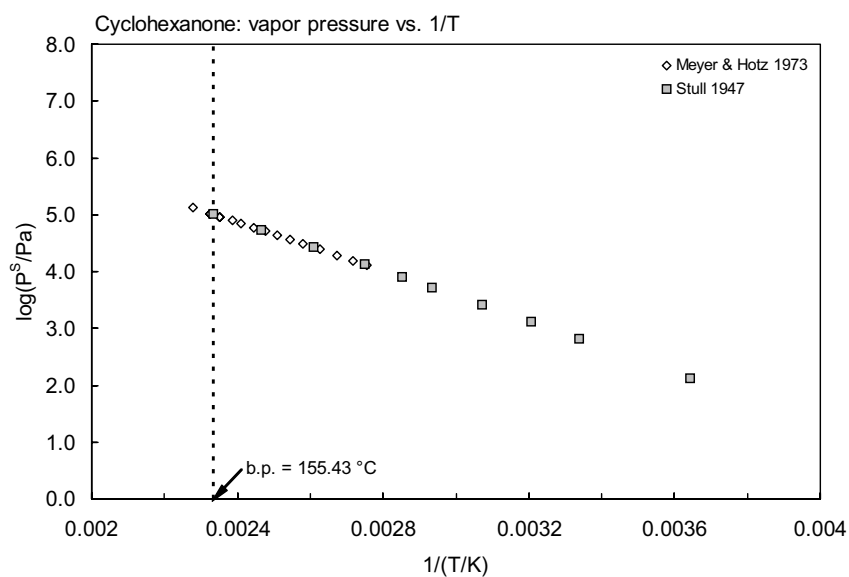
12.1.2.9   Acetophenone
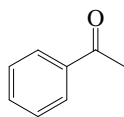
Common Name: Acetophenone
Synonym: 1-phenylethanone, methyl phenyl ketone, acetylbenzene, phenylmethylketone, hypnone
Chemical Name: acetophenone, methyl phenyl ketone
CAS Registry No: 98-86-2
Molecular Formula: C_8H_8O, $C_6H_5COCH_3$
Molecular Weight: 120.149
Melting Point (°C):
    20.5   (Stull 1947; Weast 1982–83; Lide 2003)
Boiling Point (°C):
    202   (Lide 2003)
Density (g/cm^3 at 20°C):
    1.0281   (Dreisbach 1955; Weast 1982–83; Riddick et al. 1986)
    1.02382   (25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    117.1   (calculated-density, Rohrschneider 1973)
    140.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    42.0, 53.41 (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
    16.65   (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion ΔS_{fus} (J/mol K):
    42.26   (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    5530   (shake flask-centrifuge, Booth & Everson 1948)
    6300   (shake flask-UV, Andrews & Keefer 1950)
    6022   (estimated, McGowan 1954)
    5540   (24°C, shake flask-LSC, Means et al. 1980)
    5500   (Verschueren 1983; Dean 1985, 1992)
    6130   (Southworth & Keller 1986)
    5620*   (19.9°C, shake flask-GC/TC, measured range 19.9–80.1°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
    designated * are compiled at the end of this section):
    266.6*   (50.2°C, static method-manometer, measured range 50.2–201.5°C, Kahlbaum 1898)
    66.21*   (extrapolated-regression of tabulated data, temp range 37.1–202.4°C, Stull, 1947)
    49.53   (calculated-Antoine eq., Dreisbach 1955)
    log (P/mmHg) = 7.15738 – 1723.46/(201.0 + t/°C); temp range 102–330°C (Antoine eq. for liquid state,
        Dreisbach 1955)
    41.30   (Hoy 1970)
    log (P/mmHg) = [–0.2185 × 11731.5/(T/K)] + 8.293248; temp range 37.1–202.4°C (Antoine eq., Weast 1972–73)
    57.48   (extrapolated-Cox eq., Chao et al. 1983)
    log (P/mmHg) = [1 – 474.823/(T/K)] × 10^{0.859974 – 6.15392 × 10^{-4}·(T/K) + 6.99110 × 10^{-7}·(T/K)^2}; temp
        range 310.25–475.55 K (Cox eq., Chao et al. 1983)
    52.92   (Daubert & Danner 1985)
    40.23   (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 9.1352 – 2878.8/(T/K); temp range 20–100°C (Antoine eq., Dean 1985, 1992)

49.0   (Riddick et al. 1986)

log (P/kPa) = 6.28228 – 1723.46/(201.0 + t/°C), temp range not specify (Antoine eq., Riddick et al. 1986)

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

log (P_L/kPa) = 6.28228 – 1723.46/(–72.15 + T/K); temp range 375–603 K (Antoine eq., Stephenson & Malanowski 1987)

45.00   (selected, Mackay et al. 1992, 1995; quoted, Shiu & Mackay 1997)

log (P/mmHg) = 55.5798 – 4.5101 × 10³/(T/K) –17.284·log (T/K) + 6.4184 × 10⁻³·(T/K) + 6.5557 × 10⁻¹³·(T/K)²; temp range 293–701 K (vapor pressure eq., Yaws 1994)

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

1.082   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

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

0.921*   (25.1°C, gas stripping-GC, measured range 14.9–35°C, Betterton 1991)

0.753   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

1.080, 0.982 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)

1.06*   (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)

ln K_{AW} = –9100/(T/K) + 22.47 (EPICS-UV, temp range 5–25°C, Allen et al. 1998)

0.560   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 7.307 – 3202/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.58   (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1969, 1971; Hansch & Leo 1985)

1.58   (calculated-π const., Iwasa et al. 1965)

1.73   (shake flask-UV, Chapman et al. 1972)

1.58   (HPLC-RT correlation, Lazare et al. 1974)

1.68   (shake flask-UV, Holmes & Lough 1976)

1.66 ± 0.08 (shake flask at pH 7, Unger et al. 1978)

1.66   (Hansch & Leo 1979)

1.59   (shake flask-GC, Khan et al 1979)

1.59   (shake flask-LSC, Means et al. 1980)

1.58   (shake flask-HPLC, Nahum & Horvath 1980)

1.75   (calculated-f const., Rekker's method, Hanai et al. 1981)

1.77, 1.56   (HPLC-k′ correlation, McDuffie 1981)

1.80   (HPLC-RT correlation, Hammers et al. 1982)

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

1.56   (RP-HPLC-k′ correlation, Miyake & Terada 1982)

1.63   (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

1.65   (inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)

1.65; 1.68 ± 0.02 (selected best lit. value; exptl.-ALPM, Garst & Wilson 1984)

1.59; 1.72   (HPLC-RT correlation; HPLC average, Eadsforth 1986)

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

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

1.60   (shake flask-CPC, Berthod et al. 1988)

1.58   (RP-HPLC-k′ correlation, Minick et al. 1988)

1.63   (recommended, Sangster 1989, 1993)

1.59   (CPC centrifugal partition chromatography, Gluck & Martin 1990)

1.56   (shake flask-UV spec., Alcorn et al. 1993)

1.58   (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.699–0.954 (estimated-K_{OW} and S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

1.544	(average of 3 sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
1.380	(calculated, Means et al. 1980)
1.89	(calculated-MCI χ, Gerstl & Helling 1987)
1.630	(soil, quoted, Sabljic 1987)
1.73	(RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
1.34–2.43	(soils and sediments, quoted exptl. and estimated values, Howard 1993)
1.26	(calculated-K_{OW}, Kollig 1993)
1.54	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.79, 1.63	(RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
1.61, 1.50, 1.80	(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
1.56, 1.55	(sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

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

Volatilization: based on calculated Henry's law constant, $t_{1/2}$ ~ 3.8 d from a model river of 1-m deep flowing at 1 m s^{-1} with a wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

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

k_{OH} = (2.74 ± 0.15) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1989)

k_{OH}(calc) = 1.61 × 10^{-12} cm^3 molecule^{-1} s^{-1} estimated from Atmospheric Oxidation Program; k_{OH}(exptl) = 2.74 × 10^{-12} cm^3 molecule^{-1} s^{-1} estimated from Fate of Atmospheric Pollutants Program with OH radical in vapor phase (Meylan & Howard 1993)

k_{OH}(calc) = 0.74 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(exptl) = 2.74 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant k = 0.029–0.042 h^{-1} in 30 mg L^{-1} activated sludge after a time lag of 15–20 h (Urano & Kato 1986b);

rate constants: k = 0.022 d^{-1} in ground water, k = 0.083 d^{-1} in river waters and k = 0.155 d^{-1} in Superior harbor waters (Vaishnav & Babeu 1987).

Biotransformation:

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

Half-Lives in the Environment:

Air: estimated photooxidation $t_{1/2}$ ~ 22 d in atmosphere, based on the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson 1988; quoted, Howard 1993);

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

Surface water: biodegradation $t_{1/2}$ = 8 d in river water and $t_{1/2}$ = 4.5 d in lake water (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993) and $t_{1/2}$ = 4 d in Superior harbor waters (Vaishnav & Babeu 1987).

Ground water: biodegradation $t_{1/2}$ = 32 d (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993); estimated $t_{1/2}$ ~ 0.01 yr at Noordwijk (Zoeteman et al. 1981).

Sediment:

Soil:

Biota:

TABLE 12.1.2.9.1
Reported aqueous solubilities and Henry's law constants of acetophenone at various temperatures

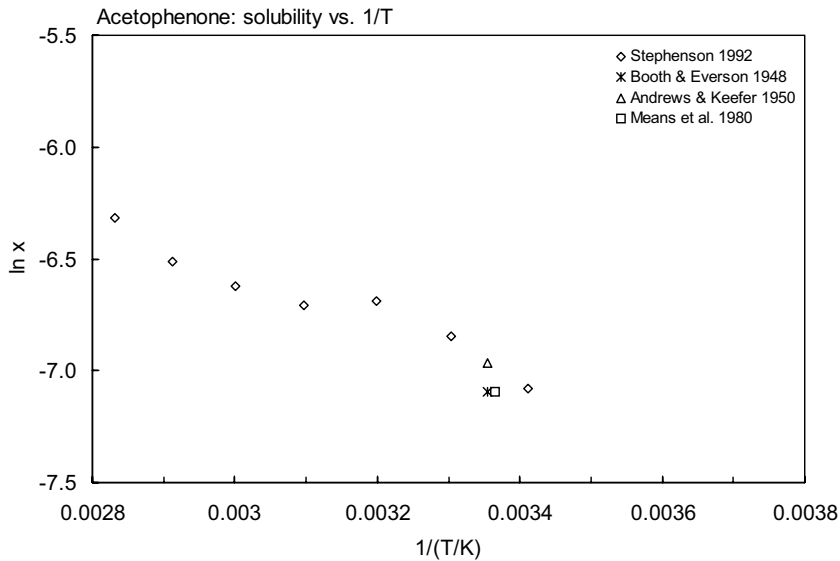| Aqueous solubility			Henry's law constant			
Stephenson 1992			Betterton 1991		Allen et al. 1998	
shake flask-GC/TC			gas stripping-GC		EPICS-UV	
t/°C	S/g·m⁻³		t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
19.9	5620		14.9	0.582	15	0.263
29.5	7100		25.1	0.921	17.5	0.362
39.5	8330		35.0	2.068	20	0.463
49.8	8140		45.0	4.053	25	1.065
60.1	8880					
70.2	9920		$\Delta H/(\text{kJ mol}^{-1}) = -50.5$		$\ln K_{AW} = A - B/(T/K)$	
80.1	12040				eq. 1	K_{AW}
					A	-9100
					B	22.47
					$\Delta H/(\text{kJ mol}^{-1}) = -75.6$	
					$\Delta S/(\text{J K}^{-1} \text{mol}^{-1}) = 186.9$	

FIGURE 12.1.2.9.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for acetophenone.

TABLE 12.1.2.9.2
Reported vapor pressures of acetophenone at various temperatures and the coefficients for the vapor pressure equations

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

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

| Kahlbaum 1898		Stull 1947	
static method-manometer*		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
50.2	266.6	37.1	133.3
56.0	400.0	64.0	666.6
61.0	533.3	78.0	1333
65.0	666.6	92.4	2666
79.0	1333.2	109.4	5333
87.3	1999.8	119.8	7999
93.4	2666.4	133.6	13332
102.4	3999.7	154.2	26664
109.7	5332.9	178.0	53329
114.7	6666.1	202.4	101325
125.2	9999.2		
133.2	13332	mp/°C	20.5
154.1	26664		
167.6	39997		
177.7	53329		
185.7	66661		
192.5	79993		
198.5	93326		
201.5	101325		

*complete list see ref.
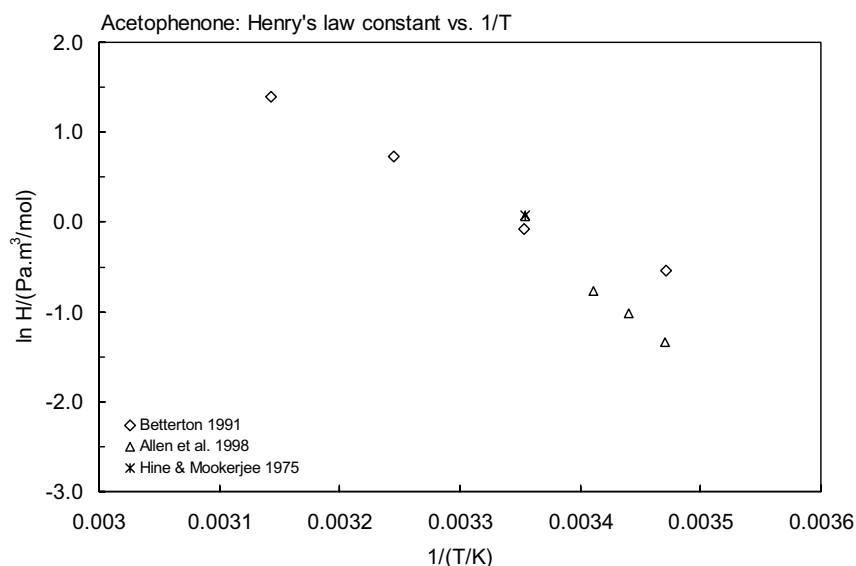
FIGURE 12.1.2.9.2 Logarithm of Henry's law constant versus reciprocal temperature for acetophenone.
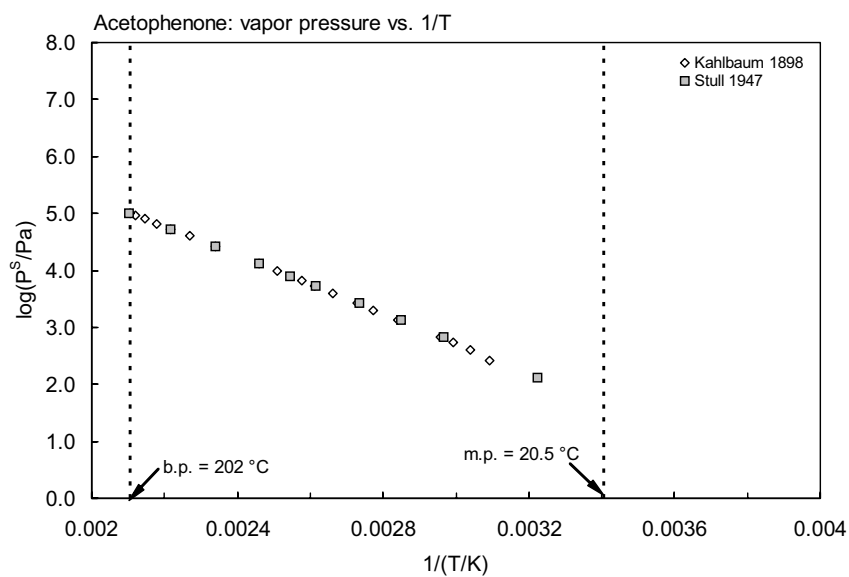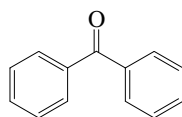
FIGURE 12.1.2.9.3 Logarithm of vapor pressure versus reciprocal temperature for acetophenone.

12.1.2.10 Benzophenone

Common Name: Benzophenone
Synonym: diphenyl ketone, diphenyl methanone
Chemical Name: benzophenone, diphenyl ketone
CAS Registry No: 119-61-9
Molecular Formula: $C_{13}H_{10}O$, $C_6H_5COC_6H_5$
Molecular Weight: 182.217
Melting Point (°C):
     48.1   (α, Weast 1982–83; Dean 1985)
     26.0   (β, Weast 1982–83; Dean 1985)
     47.9   (Lide 2003)
Boiling Point (°C):
     305.4   (Lide 2003)
Density (g/cm³ at 20°C):
     1.6077   (α, 19°C, Weast 1982–83)
     1.6059   (β, 23°C, Weast 1982–83)
     1.111   (18°C, Lide 2003)
Molar Volume (cm³/mol):
     206.8   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     53.38, 81.90   (normal bp, 25°C, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     16.99   (Dreisbach 1955)
     13.36   (Yalkowsky & Valvani 1980)
Entropy of Fusion ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} =56 J/mol K), F: 0.596 (mp at 47.9°C)

Water Solubility (g/m³ or mg/L at 25°C):
     20720, 21000   (calculated-ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)
     276   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)
     77.7   (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
     33330*   (257.15°C, temp range 257.15–302.85°C, Jaquerod & Wassher 1904; quoted, Boublik et al. 1984)
     0.617*   (extrapolated-regression tabulated data, temp range 108.3–305.5°C, Stull 1947)
     $\log (P/mmHg) = 7.81086 – 2643.0/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
     6287*   (200.50°C, ebulliometry, measured range 200.50–306.1°C, Dreisbach & Shrader 1949)
     1.242   (calculated by formula, Dreisbach 1955)
     $\log (P/mmHg) = 7.28937 – 2144.6/(181.0 + t/°C)$; temp range 1980–600°C (Antoine eq. for liquid state, Dreisbach 1955)
     $\log (P/mmHg) = [–0.2185 \times 14725.4/(T/K)] + 8.456678$; temp range 108.2–305.4°C (Antoine eq., Weast 1972–73)
     3.146*   (55.9°C, effusion method, measured range 55.9–71.2°C, DePablo 1976)
     0.086, 0.0115 (extrapolated-Antoine eq., Boublik et al. 1984)
     $\log (P/kPa) = 6.2931 – 2056.386/(173.545 + t/°C)$, temp range 200.5–306.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
     $\log (P/kPa) = 6.37814 – 2127.915/(181.209 + t/°C)$, temp range 257.1–302.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.080 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.34966 – 2331.4/(195.0 + t/°C), temp range 48–202°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.16294 – 2051.855/(173.074 + t/°C); temp range 200–306°C (Antoine eq., Dean 1985, 1992)

0.086, 0.095 (interpolated-eq.-I and II, Stephenson & Malanowski 1987)

log (P_S/kPa) = 12.44989 – 4924.329/(T/K); temp range 293–318 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P_S/kPa) = 11.736 – 4698/(T/K); temp range 298–318 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.41427 – 2144.6/(–92.15 + T/K); temp range 433–673 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

log (P/mmHg) = 16.4144 – 3.8064 × 10^3/(T/K) – 2.3984·log (T/K) – 7.4544 × 10^{-4}·(T/K) + 2.9345 × 10^{-7}·(T/K)^2; temp range 321–816 K (vapor pressure eq., Yaws 1994)

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

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

3.18	(shake flask-UV, Leo et al. 1971)
3.58	(shake flask-UV, Holmes & Lough 1976)
3.10	(shake flask-UV, Unger & Chiang 1981)
3.02	(HPLC-k′ correlation, McDuffie 1981)
3.03	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
3.18	(recommended, Sangster 1989, 1993)
3.18	(recommended, Hansch et al. 1995)
3.09	(microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)
3.32	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

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

Half-Lives in the Environment:

TABLE 12.1.2.10.1

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

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

Jaquerod & Wassher 1904		Stull 1947		Dreisbach & Shrader 1949		DePablo 1976	
in Boublik et al. 1984#		summary of lit. data		ebulliometry		effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
257.15	33330	108.2	133.3	200.50	6287	55.9	3.146
260.05	35997	141.7	666.6	206.42	7605	60.7	4.280
265.56	41330	157.6	1333	211.76	8851	66.9	7.146
270.65	46663	175.8	2666	215.46	10114	71.2	9.533
275.23	51996	195.7	5333	231.57	16500		
280.40	58662	208.2	7999	266.87	42066		
285.11	65328	224.4	13332	287.23	67661		
290.26	73327	249.8	26664	306.1	101325		
295.00	81326	276.8	53329				
300.11	91992	305.4	101325				
302.85	95992			Antoine eq. given by			
		mp/°C	48.5	Dreisbach & Martin 1949			
complete data set see ref.				Eq. 2	P/mmHg		
				A	7.81086		
eq. in Boublik et al. 1984				B	2643.0		
eq. 2	P/kPa			C	230		
A	6.37841						
B	2127.915			bp/°C	306.10		
C	181.209			mp/°C	47.93		
bp/°C	3035.428						

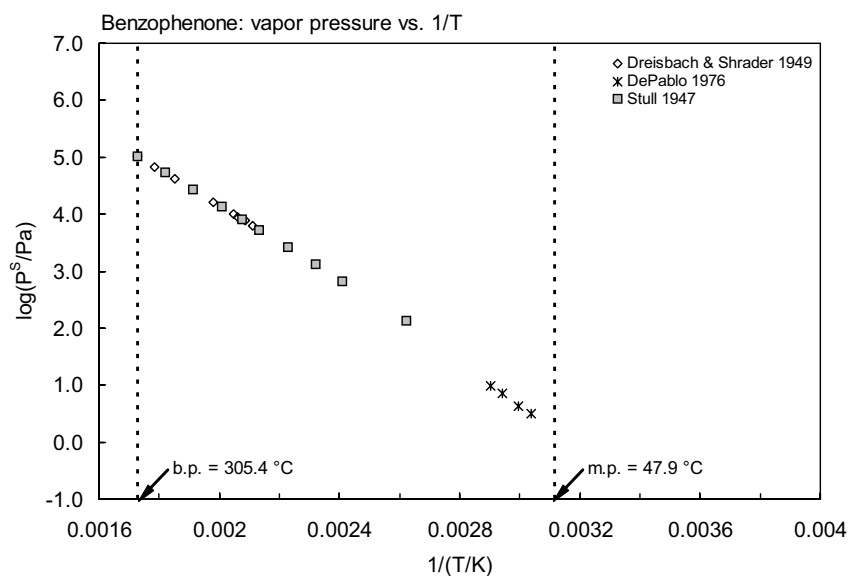# Jaquerod, A. Wassher, E. Ber. 3, 2531 (1904)

FIGURE 12.1.2.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzophenone.

12.2 SUMMARY TABLES AND QSPR PL OTS

TABLE 12.2.1
Summary of physical properties of aldehydes and ketones

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol	
							MW/ρ at 20°C	Le Bas cm³/mol
Aldehydes:								
Methanal (Formaldehyde)	50-00-0	HCHO	30.026	–92	–19.1	1		29.6
Ethanal (Acetaldehyde)	75-07-0	CH₃CHO	44.052	–123.37	20.1	1	56.23#	51.8
Propanal (Propionaldehyde)	123-38-6	C₂H₅CHO	58.079	–80	48	1	72.87	74.0
Butanal (n-Butyraldehyde)	123-72-8	C₃H₇CHO	72.106	–96.86	74.8	1	89.95	96.2
Isobutraldehyde	78-84-2	iC₃H₇CHO	72.106	–65.9	64.5	1	91.38	96.2
Pentanal (n-Valeraldehyde)	110-62-3	C₄H₉CHO	86.132	–91.5	103	1	106.40	118.4
Hexanal	66-25-1	C₅H₁₁CHO	100.158	–56	131	1	120.17	140.6
Heptanal	111-71-7	C₆H₁₃CHO	114.185	–43.4	152.8	1	140.41**	162.8
Octanal	124-13-0	C₇H₁₅CHO	128.212		171	1	156.15	185.0
2-Propenal (Acrolein)	107-02-8	H₂C=CHCHO	56.063	–87.7	52.6	1	66.83	66.6
2-Butenal	123-73-9	CH₃CH=CHCHO	70.090	–76	102.2	1	82.30	88.8
Furfural (2-Furaldehyde)	98-01-1	C₅H₄O₂	96.085	–38.1	161.7	1	82.83	92.1
Benzaldehyde	100-52-7	C₆H₅CHO	106.122	–57.1	178.8	1	101.59	118.2
Ketones:								
Acetone	67-64-1	CH₃COCH₃	58.079	–94.7	56.05	1	73.53	74.0
2-Butanone (Methyl ethyl ketone)	78-93-3	C₂H₅COCH₃	72.106	–86.64	79.59	1	89.53	96.2
2-Pentanone	107-87-9	C₃H₇COCH₃	86.132	–76.8	102.26	1	106.81	118.4
3-Pentanone	96-22-0	CH₃CH₂COCH₂CH₃	86.132	–39	101.7	1	105.77	118.4
Methyl isobutyl ketone (MIBK)	108-10-1	(CH₃)₂CHCH₂COCH₃	100.158	–84	116.5	1	125.04	140.6
2-Hexanone	591-78-6	C₄H₉COCH₃	100.158	–55	127.6	1	123.45	140.6
2-Heptanone	110-43-0	CH₃(CH₂)₄COCH₃	114.185	–35	151.05	1	140.04	162.8
2-Octanone	111-13-7	C₇H₁₆CO	128.212	–16	172.5	1	156.36	185.0
Cyclopentanone	120-92-3	C₄H₈CO	84.117	–51.90	130.57	1	88.67	99.5
Cyclohexanone	108-94-1	C₅H₁₀CO	98.142	–27.9	155.43	1	103.83	118.2
Acetophenone	98-86-2	C₆H₅COCH₃	120.149	20.5	202	1	116.87	140.4
Benzophenone	119-61-9	C₆H₅COC₆H₅	182.217	47.9	305.4	0.596	164.01#	206.8

* Assuming ΔS_{fus} = 56 J/mol K; # at 18°C; ** at 25°C.

TABLE 12.2.2
Summary of selected physical-chemical properties of aldehydes and ketones at 25°C

Compound	Solubility		Vapor pressure		log K_{OW}	Henry's law constant H/(Pa·m³/mol)				
	S/(g/m³)	C_L/(mol/m³)	P_S/Pa	P_L/Pa		calcd P/C	exptl (a)	exptl (b)	exptl (c)	exptl (c)
Aldehydes:										
Methanal	miscible	miscible	517000	517000	0.35			0.0298		0.0341
Ethanal	miscible	miscible	121300	121300	0.45		6.69	6.80	8.00	8.90
Propanal	310000	5338	42400	42400	0.59	7.944	7.44	8.40	7.51	
Butanal	71000	984.7	15200	15200	0.88	15.44	11.65	11.65		
n-Valeraldehyde			2180	2180			14.87	15.59		
Hexanal	5020	50.12			1.78		21.57	19.49		
2-Propenal (Aroclein)	208000	3710	36500	36500	–0.10	9.838	13.37		13.17	
2-Butenal	15600	222.6	5100	5100		22.91				
Furfural	79400	826.4	310	310	0.41	0.3751				
Benzyldehyde	3000	28.27	174	174	1.48	6.155	2.28			2.71
Ketones:										
Acetone	miscible	miscible	30806	30800	–0.24		3.97		3.93	3.07
2-Butanone	240000	3328.4	12100	12100	0.29	3.635	9.71		5.76	
2-Pentanone	59500	690.8	4720	4720	0.84	6.833	6.44			
3-Pentanone	34000	394.7	4700	4700	0.82	11.91				
Methyl isobutyl ketone	17000	169.7	2600	2600		15.32				
2-Hexanone	17500	174.7	1600	1600	1.38	9.157				
2-Heptanone	4300	37.66	500	500	2.08	13.28	14.73			
2-Octanone	1130	8.814	180	180	2.37	20.42	19.09			
Cyclopentanone			1540	1540						
Cyclohexanone	23000	234.4	620	620	0.81	2.646				
Acetophenone	5500	45.78	45	45	1.63	0.983				0.92
Benzophenone	276	2.541	0.09	0.151	3.18	0.059				

(a) Butler et al. 1935, Buttery et al. 1969; (b) Zhou & Mopper 1990; (c) Snider & Dawson 1985; (d) Betterton & Hoffmann 1988.

TABLE 12.2.3
Suggested half-life classes for aldehydes and ketones at various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aldehydes:				
Methanal (Formaldehyde)	1	3	3	4
Ethanal (Acetaldehyde)	1	3	3	4
Propanal (Propionaldehyde)	1	3	3	4
Butanal (*n*-Butyraldehyde)	1	3	3	4
2-Propenal (Acrolein)	1	3	3	4
2-Butenal	1	3	3	4
Furfural (2-Furaldehyde)	1	3	3	4
Benzaldehyde	1	3	3	4
Ketones:				
Acetone	4	3	4	5
2-Butanone (Methyl ethyl ketone)	4	3	3	5
2-Pentanone	3	4	4	5
3-Pentanone	3	4	4	5
Methyl isobutyl ketone (MIBK)	3	4	4	5
2-Hexanone	3	4	4	5
2-Heptanone	3	4	4	5
Cyclohexanone	3	4	4	5
Acetophenone	5	4	4	5
Benzophenone	5	4	4	5

where,

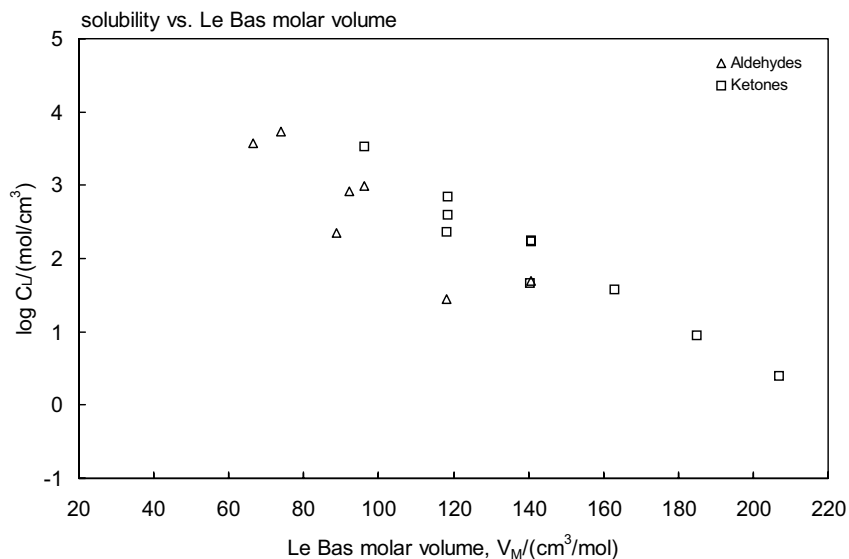| Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

FIGURE 12.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.
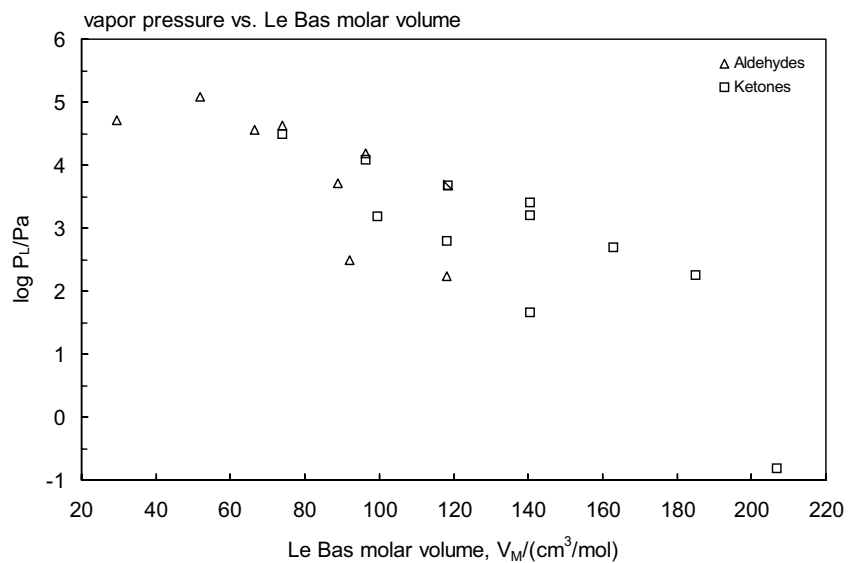

FIGURE 12.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.
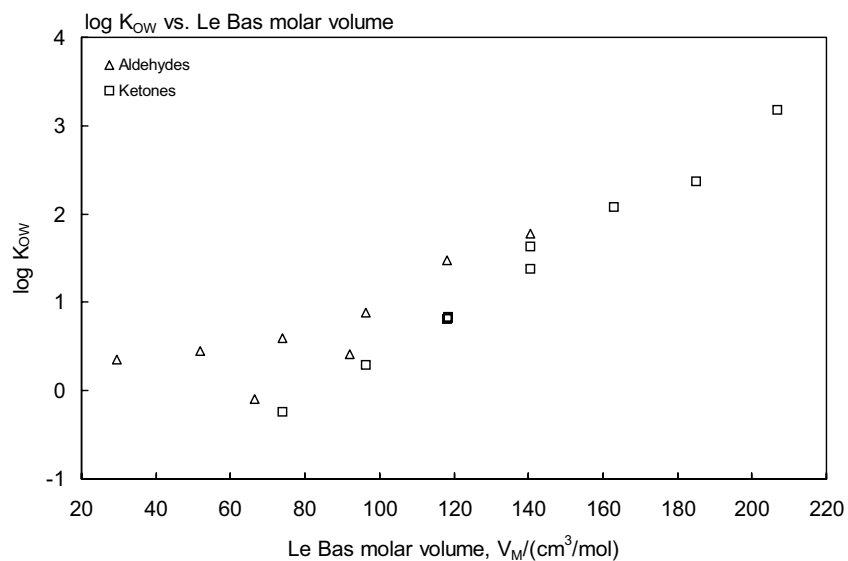
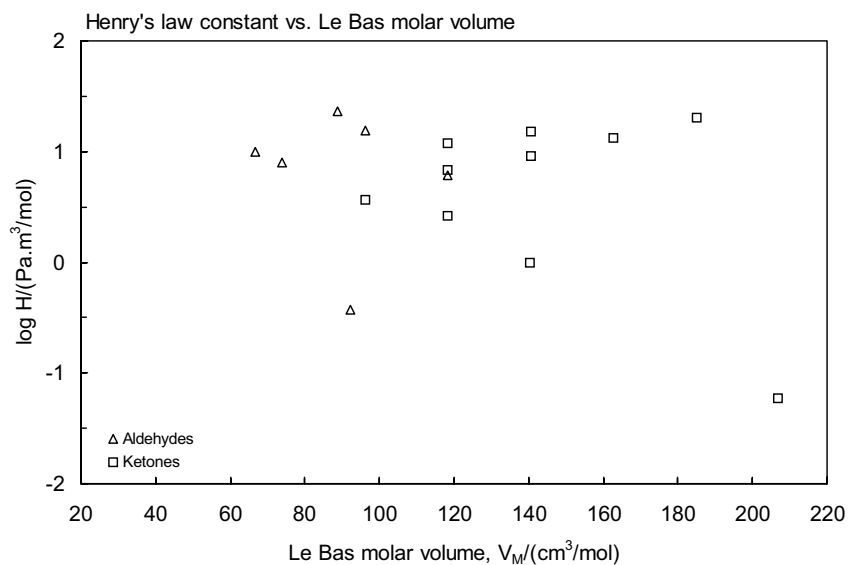**FIGURE 12.2.3** Octanol-water partition coefficient versus Le Bas molar volume for aldehydes and ketones.

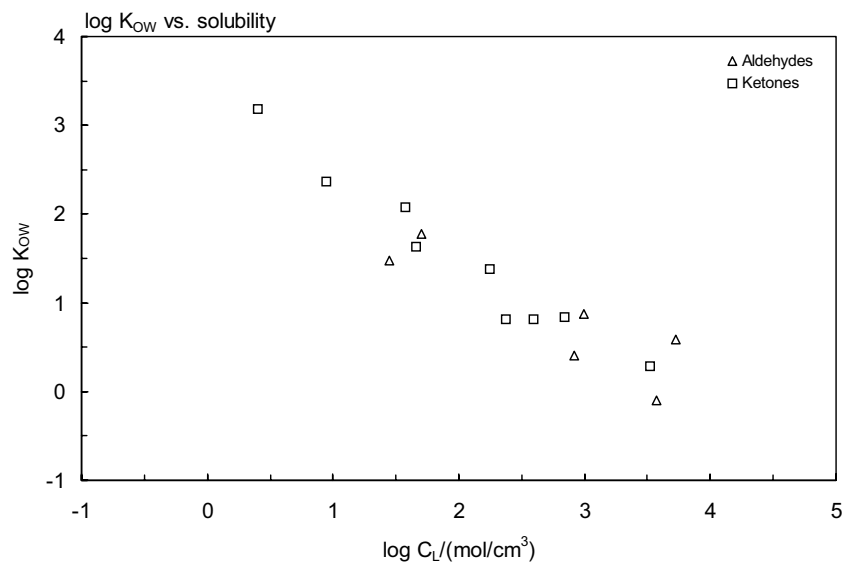**FIGURE 12.2.4** Henry's law constant versus Le Bas molar volume for aldehydes and ketones.

FIGURE 12.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aldehydes and ketones.

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