2 Aliphatic and Cyclic Hydrocarbons

CONTENTS

2.1   LIST OF CHEMICALS AND DATA COMPILATIONS

2.1.1   SATURATED HYDROCARBONS

2.1.1.1   Alkanes

2.1.1.1.1   Isobutane (2-Methylpropane)

Common Name: Isobutane
Synonym: 2-methylpropane
Chemical Name: 2-methylpropane
CAS Registry No: 75-28-5
Molecular Formula: C_4H_{10}
Molecular Weight: 58.122
Melting Point (°C):
   –159.4   (Weast 1984; Lide 2003)
Boiling Point (°C):
   –11.73   (Lide 2003)
Density (g/cm³ at 20°C):
   0.5490   (Weast 1984)
   0.5571, 0.5509   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
   105.9   (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
   96.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   19.121, 21.297 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   4.540   (Dreisbach 1959; Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   48.9   (shake flask-GC at atmospheric pressure, McAuliffe 1963, 1966)

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.):
   101783*   (–11.609°C, static method-manometer, measured range –85.5 to –11.609°C, Aston et al. 1940)
   101325*   (–11.7°C, summary of literature data, temp range –109.2 to –11.7°C, Stull 1947)
   348100   (calculated from determined exptl. data, Dreisbach 1959)
   log (P/mmHg) = 6.74808 – 882.80/(240.0 + t/°C); temp range –75 to 30°C (Antoine eq. for liquid state, Dreisbach 1959)
   357000   (interpolated-Antoine eq., temp range –86.57 to 18.88°C, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C); temp range –86.57 to 18.88°C (Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = [–0.2185 × 5084.4/(T/K)] + 7.250; temp range –115 to –34°C (Antoine eq., Weast 1972–73)
   log (P/mmHg) = [–0.2185 × 5416.2/(T/K)] + 7.349085; temp range –109.5 to 137.5°C (Antoine eq., Weast 1972–73)
   312486, 313702* (21.07, 21.22°C, vapor-liquid equilibrium, measured range 4.580–71.17°C, Steele et al. 1976)
   356600   (extrapolated-Antoine eq., temp range –87 to 7°C, Dean 1985, 1992)
   log (P/mmHg) = 6.90148 – 946.35/(246.68 + t/°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
   log (P/kPa) = 6.00272 – 947.54/(248.87 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
   351130   (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.03538 - 946.35/(-26.47 + T/K)$; temp range 186–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 7.83572 - 1470.08/(3.99 + T/K)$; temp range 121–187 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.93028 - 907.164/(-30.14 + T/K)$; temp range 263–306 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.26924 - 1102.296/(-2.12 + T/K)$; temp range 301–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.95371 - 1648.648/(77.939 + T/K)$; temp range 361–408 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P/mmHg) = 31.2541 - 1.9532 \times 10^3/(T/K) - 8.806 \cdot \log (T/K) + 8.9246 \times 10^{-11} \cdot (T/K) + 5.7501 \times 10^{-6} \cdot (T/K)^2$; temp range 114–408 K (vapor pressure eq., Yaws 1994)

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

118640	(converted from $1/K_{AW} = C_W/C_A$ reported as exptl., Hine & Mookerjee 1975)
100980, 22090	(calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
120000	(calculated-P/C, Mackay & Shiu 1981)
116700	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.76	(shake flask-GC, Leo et al. 1975)
2.76	(recommended, Sangster 1993)
2.76	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH}*(exptl) $= 1.42 \times 10^{12}$ cm^3 mol^{-1} s^{-1}, k_{OH}(calc) $= 1.31 \times 10^{12}$ cm^3 mol^{-1} s^{-1} at 297 K, measured range 297–499 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{OH} = 1.28 \times 10^9$ L mol^{-1} s^{-1} at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)

$k_{OH} = (2.52 \pm 0.05) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

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

$k_{OH} = (2.29 \pm 0.06) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

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

k_{OH}* $= 2.34 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

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

k_{NO3}* $= (1.10 \pm 0.2) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–523 K, atmospheric $t_{\frac{1}{2}} = 1750$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)

$k_{OH} = 7.38 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 6.50 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

$k_{NO3} = 9.8 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1991)

$k_{OH} = 2.34 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and an estimated lifetime was 59 h (Altshuller 1991)

k_{NO3}(exptl) $= 9.8 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(recommended) $= 9.9 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) $= 7.90 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* $= 2.19 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}* $= 10.6 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ = 1750 h due to reaction with NO_3 radical during the night at room temp., and $t_{1/2}$ = 82 h for reaction with OH radical (Bagley et al. 1990);

   atmospheric lifetime was estimated to be 59 h, based on a photooxidation rate constant k = 2.34×10^{-12} cm^3 $molecule^{-1}$ s^{-1} in summer daylight with OH radical (Altshuller 1991).

TABLE 2.1.1.1.1.1

Reported vapor pressures of isobutane (2-methylpropane) 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)	

Aston et al. 1940		Stull 1947		Steele et al. 1976	
static method-manometer		summary of literature data		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–85.5	1516	–109.2	133.3	4.580	183196
–71.704	4261	–91.1	666.6	4.620	185019
–56.431	11579	–86.4	1333	21.07	312486
–44.107	23233	–77.9	2666	21.22	313702
–27.576	52132	–68.4	5333	37.55	497811
–22.071	66405	–62.4	7999	37.62	498721
–18.761	76349	–51.4	13332	54.43	762470
–13.328	95476	–41.5	26664	54.50	763484
–11.609	101783	–27.1	53329	71.06	1112244
		–11.7	101325	71.17	1114778
mp/°C	–145	mp/°C	–145		
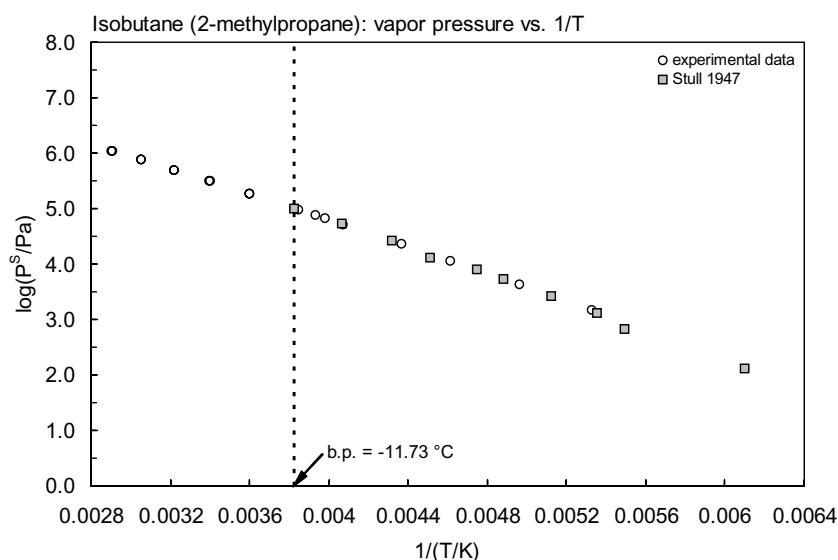
FIGURE 2.1.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for isobutane.

2.1.1.1.2   2,2-Dimethylpropane (Neopentane)

Common Name: 2,2-Dimethylpropane
Synonym: neopentane, tetramethylmethane
Chemical Name: 2,2-dimethylpropane
CAS Registry No: 463-82-1
Molecular Formula: C_5H_{12}
Molecular Weight: 72.149
Melting Point (°C):
    –16.4   (Lide 2003)
Boiling Point (°C):
    9.503   (Dreisbach 1959; Stephenson & Malanowski 1987)
    9.48   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.5910, 0.5852   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    122.10   (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992)
    117.6   (20°C, Stephenson & Malanowski 1987)
    118.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    21.778, 22.753   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    3.255   (Dreisbach 1959; Chickos et al. 1999)
    3.146   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    12.69   (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    33.2   (shake flask-GC at 1 atmospheric pressure, McAuliffe 1966)

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.):
    177930*   (Antoine eq. regression, temp range –112 to 9.8°C, Stull 1947)
    171350   (calculated from determined data, Dreisbach 1959)
    $\log (P/\text{mmHg}) = 6.73812 – 950.84/(237.0 + t/°C)$; temp range –60 to 55°C (Antoine eq. for liquid state, Dreisbach 1959)
    171586*   (derived from compiled data, temp range –13.729 to 29.914°C, Zwolinski & Wilhoit 1971)
    $\log (P_S/\text{mmHg}) = 7.2034 – 1020.7/(230.0 + t/°C)$; temp range –52 to 17.6°C (Antoine eq., solid, Zwolinski & Wilhoit 1971)
    $\log (P_L/\text{mmHg}) = 6.60427 – 883.42/(227.782 + t/°C)$; temp range –13.729 to 29.914°C (Antoine eq., liquid, Zwolinski & Wilhoit 1971)
    $\log (P/\text{mmHg}) = [–0.2185 \times 5648.6/(T/K)] + 7.263947$; temp range –102 to 152.5°C (Antoine eq., Weast 1972–73)
    169019*   (24.56°C, ebulliometry, measured range –5.128 to 40°C, Osborn & Douslin 1974)
    $\log (P/\text{mmHg}) = 6.60427 – 883.42/(227.78 + t/°C)$; temp range –14 to 29°C (Antoine eq., Dean 1985, 1992)
    171300   (selected, Riddick et al. 1986)
    $\log (P/\text{kPa}) = 6.89316 – 938.234/(235.249 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
    171520, 171450   (interpolated-Antoine eq.-III and IV, Stephenson & Malanowski 1987)
    $\log (P_S/\text{kPa}) = 6.3283 – 1020.7/(–43.15 + T/K)$; temp range 223–256 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P_S/kPa) = 7.07825 – 1372.459/(–8.39 + T/K); temp range 223–256 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.76532 – 900.545/(–43.111 + T/K); temp range 268–313 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.83935 – 937.641/(–38.071 + T/K); temp range 257–315 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.08953 – 1080.237/(–17.896 + T/K); temp range 312–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.26795 – 2114.713/(128.175 + T/K); temp range 382–433 K (Antoine eq-VI, Stephenson & Malanowski 1987)

log $(P/mmHg)$ = 26.6662 – 1.9307×10^3/(T/K) – 7.0448·log (T/K) + 7.4104×10^{-9}·(T/K) + 3.9463×10^{-6}·(T/K)^2; temp range 257–434 K (vapor pressure eq., Yaws 1994)

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

221000	(calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
125640, 334380	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
373000	(calculated-P/C, Mackay & Shiu 1981)
213250	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.11	(shake flask-GC, Leo et al. 1975; Leo et al. 1971; Hansch & Leo 1979)
2.95, 3.41, 3.22	(calculated-fragment const., Rekker 1977)
3.30, 3.08	(calculated-MO, calculated-π const., Bodor et al. 1989)
3.11	(recommended, Sangster 1989, 1993)
2.98	(calculated-V_M, Wang et al. 1992)
3.11	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

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

k_{OH}*(exptl) = 6.50×10^{12} cm^3 mol^{-1} s^{-1}, k_{OH}(calc) = 5.27×10^{12} cm^3 mol^{-1} s^{-1} at 298 K, measured range 298–493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{OH}(exptl) = 6.50×10^{11} cm^3 mol^{-1} s^{-1}, k_{OH}(calc) = 5.37×10^{11} cm^3 mol^{-1} s^{-1} at 298 K (Greiner 1970)

$k_{O(3P)}$ = 5.50×10^{-15} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom at room temp. (Herron & Huie 1973)

k_{OH} = $(1.04 \pm 0.17) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

k_{OH} = 9.30×10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)

k_{OH} = 9.0×10^{-13} cm^3 molecule^{-1} s^{-1} (Winer et al. 1979)

k_{OH}* = 8.49×10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990, 1991)

k_{OH}* = 8.48×10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 2.1.1.1.2.1
Reported vapor pressures of 2,2-dimethylpropane (neopentane) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$	(3)	
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	
$\log P = A[1 - \Phi/(T/K)]$	(5)	where $\log A = a + b(T/K) + c(T/K)^2$

Stull 1947		Zwolinski & Wilhoit 1971				Osborn & Douslin 1974	
summary of literature data		selected values				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
			solid		liquid		
−102.0	133.3	−52.0	4000	−13.729	39997	−5.128	57818
−85.4	666.6	−48.0	5333	−7.047	53329	−0.301	70121
−76.7	1333	−45.0	6666	−1.570	66661	4.577	84666
−67.2	2666	−41.9	7999	3.112	79993	9.500	101325
−56.1	5333	−37.4	10666	7.224	93326	14.472	120793
−49.0	7999	−33.8	13332	7.991	95992	19.492	143246
−39.1	13332	−27.0	19998	8.742	98659	24.560	169019
−23.7	26667	−21.8	26664	9.112	101325	29.675	198488
−7.10	53329	−17.6	33331	10.199	103991	34.838	232017
9.50	101325			10.906	106658	40.048	270022
		bp/°C	9.478	14.251	119990		
mp/°C	−16.6	Antoine eq.		17.324	133322	Cox eq.	
		eq. 2	P/mmHg	22.829	159987	eq. 5	P/mmHg
		A	7.2034	29.914	199984	Φ	282.650
		B	1020.7	25.0	171586	a	0.802264
		C	230.0			b	-6.70026×10^{-4}
		temp range −52 to −17.6°C		Antoine eq.		c	11.22918×10^{-7}
		pres. range 30–250 mmHg		eq. 2	P/mmHg	for temp range 268–314 K	
				A	6.60427		
		$\Delta H_V/(kJ \, mol^{-1})$ =		B	883.42		
		at 25°C	21.85	C	227.782		
		at bp	22.75	temp range −14 to 30°C			
				pressure 300–1800 mmHg			
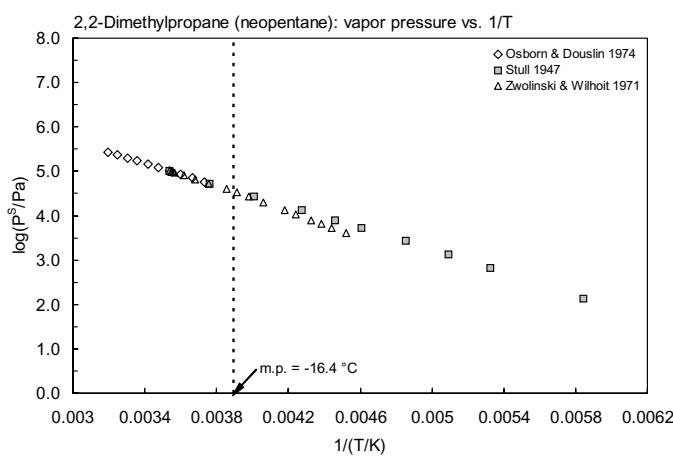
FIGURE 2.1.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2,2-dimethylpropane.

2.1.1.1.3   n-Butane

Common Name: *n*-Butane
Synonym: 1-butane
Chemical Name: *n*-butane
CAS Registry No: 106-97-8
Molecular Formula: C_4H_{10}
Molecular Weight: 58.122
Melting Point (°C):
    –138.3   (Lide 2003)
Boiling Point (°C):
    –0.50   (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
    0.5788, 0.5730   (20°C, 25°C, Dreisbach 1959)
    0.5786, 0.5729   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    100.45, 101.45   (20°C, 25°C, calculated-density)
    96.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    21.066, 22.393   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    4.393   Parks & Huffman 1931)
    4.661   (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    34.56   (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    65.6   (shake flask-UV, Morrison & Billett 1952)
    67.0   (shake flask-UV, Claussen & Polglase 1952)
    72.7   (shake flask-GC, Franks et al. 1966)
    61.4   (shake flask-GC, McAuliffe 1963, 1966)
    61.66   (shake flask-GC, Coates et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    288200   (extrapolated-Antoine eq. regression, temp range –101.5 to –0.5°C, Stull 1947)
    243050   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.83029 – 945.9/(240.0 + t/°C); temp range –60 to 30°C (Antoine eq. for liquid state, Dreisbach
        1959)
    242647   (derived from compiled data, temp range –77.62 to 18.88°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.80896 – 935.56/(238.73 + t/°C); temp range –77.62 to 18.88°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    242840   (extrapolated-Antoine eq., temp range –77 to 19°C, Dean 1985, 1992)
    log (P/mmHg) = 6.80896 – 935.86/(238.73 + t/°C); temp range –77 to 19°C (Antoine eq., Dean 1985, 1992)
    243000   (lit. average, Riddick et al. 1986)
    log (P/kPa) = 5.93266 – 935.773/(238.789 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    242810   (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.93386 – 935.86/(–34.52 + T/K); temp range 195–292 K (Antoine eq.-I, Stephenson &
        Malanowski 1987)
    log (P_L/kPa) = 7.3327 – 1409.73/(T/K); temp range 135–213 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.07512 – 1007.247/(–25.272 + T/K); temp range 273–321 K (Antoine eq.-III, Stephenson &
        Malanowski 1987)

log (P_L/kPa) = 6.32267 − 1161.1/(−3.107 + T/K); temp range 316–383 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.04942 − 1770.348/(84.979 + T/K); temp range 375–425 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P/mmHg)$ = 27.0441 − 1.9049 × 10^3/(T/K) − 7.1805·log (T/K) − 6.6845 × 10^{-11}·(T/K) + 4.219 × 10^{-6}·$(T/K)^2$; temp range 135–425 K (vapor pressure eq., Yaws 1994)

592440   (57.01°C, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)

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

94240	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
82080, 22100	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
95900	(calculated-P/C, Mackay & Shiu 1975; Mackay 1981; Mackay & Shiu 1981)
80210	(calculated-MCI χ, Nirmalakhandan & Speece 1988)
92910	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.89	(shake flask-GC, Leo et al. 1975)
2.89	(concn. ratio, Cramer 1977)
2.46, 2.84, 2.96	(calculated-f const., Rekker 1977)
2.89, 2.76	(Hansch & Leo 1979)
2.79	(calculated-hydrophobicity const., Iwase et al. 1985)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{O3} = 9.8 × 10^{-24} cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 298–323 K (Schubert & Pease 1956)

$k_{O(3P)}$ = 3.1 × 10^{-14} cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom (Herron & Huie 1973)

k_{OH} = 3.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ (Atkinson et al. 1979)

k_{OH}*(exptl) = 1.66 × 10^{12} cm³ mol⁻¹ s⁻¹, k_{OH}(calc) = 1.54 × 10^{12} cm³ mol⁻¹ s⁻¹ at 298 K, measured range 298–495 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{OH} = 1.8 × 10^9 L mol⁻¹ s⁻¹ with atmospheric $t_{1/2}$ = 2.4 to 24 h at 300 K (Darnall et al. 1976)

k_{OH} = 1.8 × 10^9 M⁻¹ s⁻¹ in polluted atmosphere at 305 ± 2 K (relative rate method, Lloyd et al. 1976)

k_{OH} = 3.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ with a loss rate at 0.11 d⁻¹ for the reaction with OH radical and an average OH concn of 1.2 × 10^6 molecules/cm³ (Zafonte & Bonamassa 1977)

k_{OH}(exptl) = (2.57 − 4.22) × 10^{-12} cm³ molecule⁻¹ s⁻¹, k_{OH}(calc) = 2.71 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at atmospheric pressure and 300 K (Darnall et al. 1978)

k_{OH} = 2.58 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 299 ± 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

k_{O3} < 10^{-23} cm³ molecule⁻¹ s⁻¹ with a loss rate of < 6 × 10^{-7} d⁻¹, k_{OH} = 2.6 × 10^{-12} cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.2 d⁻¹ and k_{NO3} = 3.6 × 10^{-17} cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.0007 d⁻¹ (Atkinson & Carter 1984; Atkinson 1985)

k_{OH}* = 2.54 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

k_{OH}* = 2.54 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K, k_{NO3} = 6.5 × 10^{-17} cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (Atkinson 1990; Altshuller 1991).

$k_{NO3}* = (0.45 \pm 0.06) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–523 K, atmospheric $t_{1/2} = 4300$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)

atmospheric lifetime was estimated to be 54 h, based on the photooxidation reaction rate constant with OH radical during summer daylight hours (Altshuller 1991)

$k_{NO3} = (\leq 2.0 – 6.6) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296–298 K (Atkinson 1991)

k_{NO3}(exptl) $= 6.70 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(recommended) $= 4.3 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296 $\pm$ 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}* = 2.44 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3}* = 4.59 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

$k_{OH}* = 2.37 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 6.5$ h in ambient air based on reaction with OH radicals at 300 K (Doyle et al. 1975);

photolysis $t_{1/2} = 2.4$ to 24 h (Darnall et al. 1976);

atmospheric lifetimes τ(calc) $= 4 \times 10^7$ h for reaction with O$_3$, $\tau = 107$ h with OH radical and $\tau = 32150$ h with NO$_3$ radical based on reaction rate constants and environmental concentrations of OH, NO$_3$ radicals and O$_3$ in the gas phase (Atkinson & Carter 1984);

atmospheric lifetimes τ(calc) $= 222$ h for the reaction with OH radical, $\tau = 4 \times 10^7$ h with O$_3$ and $\tau = 32150$ h with NO$_3$ radical based on the rate constants and environmental concentrations of OH, NO$_3$ radicals and O$_3$ in the gas phase (Atkinson 1985);

atmospheric $t_{1/2} = 4300$ h due to reaction with NO$_3$ during the night at room temp., and $t_{1/2} = 77$ h for reaction with OH radical (Bagley et al. 1990);

atmospheric lifetime $\tau \sim 54$ h based on a photooxidation reaction rate constant of 2.54×10^{-12} cm^3 molecule^{-1} s^{-1} with OH radicals during summer daylight hours (Altshuller 1991).

2.1.1.1.4   2-Methylbutane (Isopentane)

Common Name: 2-Methylbutane
Synonym: Isopentane
Chemical Name: 2-methylbutane
CAS Registry No: 78-78-4
Molecular Formula: C_5H_{12}; $CH_3CH(CH_3)CH_2CH_3$
Molecular Weight: 72.149
Melting Point (°C):
    –159.77   Lide 2003)
Boiling Point (°C): 27.875
    27.88   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6197, 0.6146   (20°C, 25°C, Dreisbach 1959)
    0.6193, 0.6142   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    116.5, 117.47   (20°C, 25°C, calculated-density)
    118.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.1505   (Dreisbach 1959, Riddick et al. 1986)
    5.13   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    45.23, 43.35 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
    47.8   (shake flask-GC, McAuliffe 1963,1966)
    46.9*   (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
    72.4; 49.6, 55.2   (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
    48.0   (shake flask-GC, Price 1976)
    48.0   (selected, Riddick et al. 1986)
    48.5*   (IUPAC recommended best value, temp range 0–60°C, Shaw 1989)
    52.11*   (calculated-liquid-liquid   equilibrium   LLE   data,   temp   range   273.2–323.2   K,
                        Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    82790   (22.04°C, Schumann et al. 1942)
    83720*   (22.44°C, manometer, temp range 16.291–28.587°C, Willingham et al. 1945)
    log (P/mmHg) = 6.87372 – 1075.816/(233.259 + t/°C); temp range 16.291–28.587°C (Antoine eq. from exptl.
        data, manometer, Willingham et al. 1945)
    99550*   (Antoine eq. regression, temp range –82.9 to 27.8°C, Stull 1947)
    91740   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.78967 – 1020.012/(223.097 + t/°C); temp range –45 to 75°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    91646*   (extrapolated-Antoine eq, temp range –67.03 to 49.14°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.83315 – 1040.73/(235.455C + t/°C); temp range –67.03 to 49.14°C (Antoine eq., Zwolinski
        & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 6470.8/(T/K)] + 7.544680; temp range: –82.9 to 180.3°C, (Antoine eq., Weast 1972–73)
    91730, 92100 (interpolated, Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.04913 – 1081.748/(239.817 + t/°C); temp range –56 to 22.4°C (Antoine eq. from reported exptl. data of Schumann et al. 1942, Boublik et al. 1984)

log (P/kPa) = 5.9333 – 1029.602/(234.294 + t/°C); temp range 16.29–28.59°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

91660   (interpolated-Antoine eq., temp range –87 to 7°C, Dean 1985)

log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)

91700   (quoted, Riddick et al. 1986)

log (P/kPa) = 5.92023 – 1022.88/(233.460 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

91640   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.95805 – 1040.73/(–37.705 + T/K); temp range 216–323 K (Antoine eq-I., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.32287 – 1279.08/(–4.481 + T/K); temp range 300–460 K (Antoine eq-II., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.39629 – 1325.048/(1.244 + T/K); temp range 320–391 K (Antoine eq-III., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.22589 – 1212.803/(–12.958 + T/K); temp range 385–416 K (Antoine eq-IV., Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.09160 – 3167.07/(233.708 + T/K); temp range 412–460 K (Antoine eq-V., Stephenson & Malanowski 1987)

log (P/mmHg) = 29.2963 – 2.1762 × 10^3/(T/K) – 7.883·log (T/K) – 4.6512 × 10^{-11}·(T/K) + 3.8997 × 10^{-6}·(T/K)^2; temp range 113–460 K (vapor pressure eq., Yaws 1994)

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

140000   (calculated-P/C, Mackay et al. 1979; Mackay 1981)

138000; 140000, 139000, 134700   (recommended; calculated-P/C, Mackay & Shiu 1981))

138210   (selected, Mills et al. 1982)

138290   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

2.41   (calculated-MCI χ, Murray et al. 1975)

2.83   (calculated-molar volume V_M, Wang et al. 1992)

2.4698   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = 2.0 × 10^{12} cm^3 mol^{-1} s^{-1} with atmospheric $t_{1/2}$ = 2.4–24 h (Lloyd 1976, Darnall et al. 1976)

k_{OH} = (3.78 ± 0.07) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

k_{OH} = (3.97 ± 0.11) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990, 1991; Altshuller 1991)

k_{NO3}* = (1.60 ± 0.2) × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–523 K, atmospheric $t_{1/2}$ = 1200 h during the night at room temp. (discharge flow system, Bagley et al. 1990)

k_{OH} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, estimated atmospheric lifetime of 36 h (Altshuller 1991)

k_{NO_3}(exptl) $= 1.56 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, k_{NO_3}(calc) $= 2.49 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH} = 3.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{NO_3}* $= 1.62 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 2.0×10^{12} cm^3 mol^{-1} s^{-1} for the reaction with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976) with atmospheric $t_{\frac{1}{2}}$ = 2.4–24 h (Darnall et al. 1976);

atmospheric $t_{\frac{1}{2}}$ = 1200 h due to reaction with NO$_3$ radical during the night at room temp., and $t_{\frac{1}{2}}$ = 50 for reaction with OH radical (Bagley et al. 1990);

atmospheric lifetime of 36 h, based on rate constant of 3.90×10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with OH radicals during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.4.1
Reported aqueous solubilities of 2-methylbutane (isopentane) at various temperatures

Pavlova et al. 1966		Polak & Lu 1973		Shaw 1989a		Mączyński et al. 2004	
in IUPAC 1989		shake flask-GC/FID		IUPAC recommended		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	46.9	0	72.4	0	72	0	68.14
40	57.7	25	49.6	20	47	20	56.12
50	70.1			25	48.5	25	52.11
60	79.3			30	51	40	52.11
				40	58	50	56.12
				50	70		
				60	79		
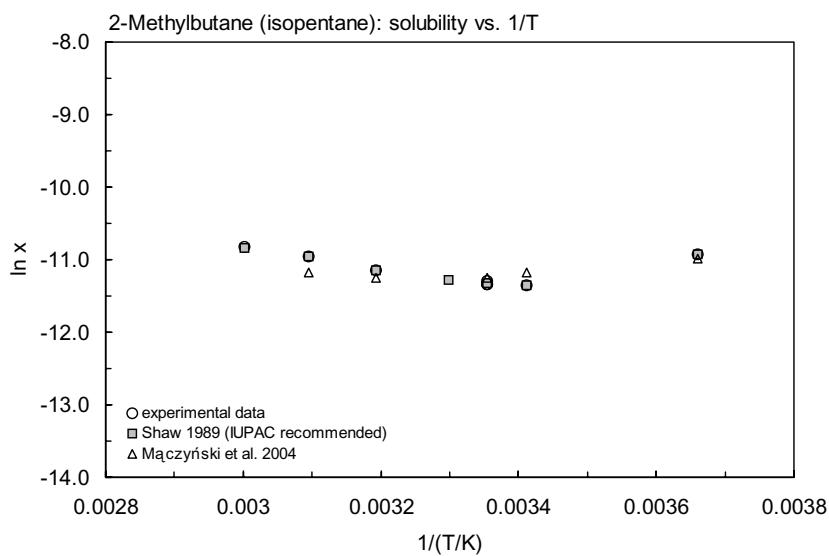
FIGURE 2.1.1.1.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methylbutane.

TABLE 2.1.1.1.4.2
Reported vapor pressures of 2-methylbutane (isopentane) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$
$$\log P = A - B/(C + t/°C) \quad (2) \qquad \ln P = A - B/(C + t/°C) \quad (2a)$$
$$\log P = A - B/(C + T/K) \quad (3) \qquad \ln P = A - B/(C + T/K) \quad (3a)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$
$$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2) \quad (5)$$

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971			
ebulliometry		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
16.291	66760	−82.9	133.3	−57.03	1333	25.517	93326
22.435	83722	−65.8	666.6	−47.32	2666	26.320	95992
26.773	97608	−57.0	1333	−41.14	4000	27.156	98659
27.24	99207	−47.3.	2666	−36.49	5333	27.875	101325
27.673	100700	−36.5	5333	−32.74	6666	25.0	91646
28.16	102402	−29.6	7999	−29.56	7999		
28.587	103922	−20.2	13332	−24.35	10666	eq. 2	P/mmHg
		−5.90	26664	−20.11	13332	A	6.83315
bp/°C	27.852	10.5	53329	−11.97	19998	B	1040.73
		27.8	101325	−5.81	26664	C	235.445
eq. 2	P/mmHg			−0.79	33331	bp/°C	28.875
A	6.78967	mp/°C	−159.7	3.47	39997	$\Delta H_V/(kJ\ mol^{-1})$ =	
B	1020.012			10.53	53329	at 25°C	24.84
C	233.097			16.293	66661	at bp	24.69
				21.208	79993		
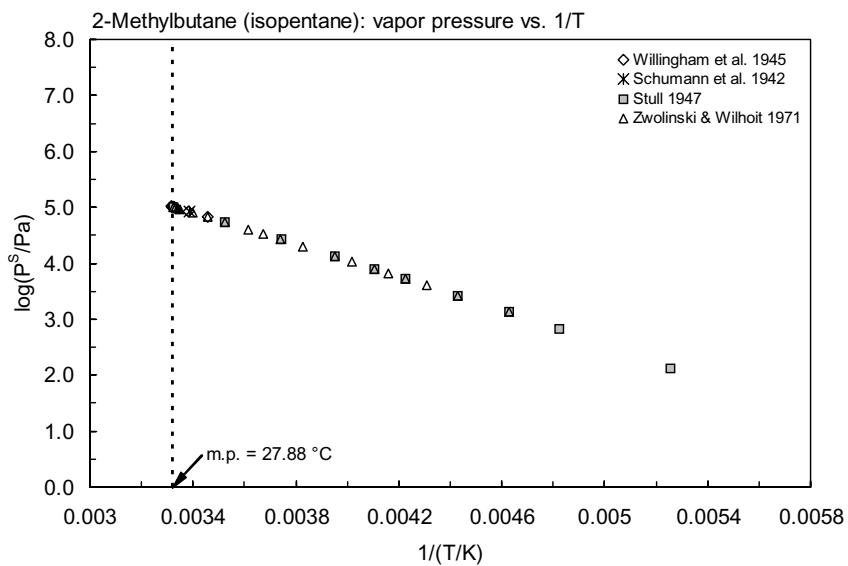
FIGURE 2.1.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylbutane.

2.1.1.1.5   2,2-Dimethylbutane

Common Name: 2,2-Dimethylbutane
Synonym: neohexane, dimethylpropylmethane
Chemical Name: 2,2-dimethylbutane
CAS Registry No: 75-83-2
Molecular Formula: C_6H_{14}; $CH_3CH(CH_3)_2CH_2CH_3$
Molecular Weight: 86.175
Melting Point (°C):
　　–99.8　　　(Lide 2003)
Boiling Point (°C):
　　49.73　　　(Lide 2003)
Density (g/cm^3 at 20°C):
　　0.6492, 0.6445 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
　　132.74, 133.71　　　(20°C, 25°C, calculated-density)
　　140.6　　　　　　　(calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
　　5.791　　　　　　(Dreisbach 1959; Riddick et al. 1986)
　　5.4, 0.28, 0.58　　(–146.35, –132.35, –98.95°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
　　45.88, 42.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
　　18.4　　　(shake flask-GC, McAuliffe 1963,1966)
　　39.4, 23.8　(0, 25°C, shake flask-GC, Polak & Lu 1973)
　　21.2　　　(shake flask-GC, Price 1976)
　　21.2　　　(shake flask-GC, Krzyzanowska, Szeliga 1978)
　　18.0　　　(selected Riddick et al. 1986)
　　21.0　　　(IUPAC recommended best value, Shaw 1989)
　　19.63　　　(calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
　　43320　　　(24.47°C, manometer, temp range 15.376–50.529°C, Willingham et al. 1945)
　　log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t/°C); temp range 15.376–50.529°C (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)
　　43480　　　(Antoine eq. regression, temp range –69.3 to 49.7°C, Stull 1947)
　　42570　　　(25°C, Nicolini & Laffitte 1949)
　　42540　　　(calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)
　　log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t/°C); temp range –25 to 95°C (Antoine eq. for liquid state, Dreisbach 1959)
　　42543　　　(interpolated-Antoine eq., temp range –41.5 to 72.8°C, Zwolinski & Wilhoit 1971)
　　log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t/°C); temp range –41.5 to 72.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
　　log (P/mmHg) = [–0.2185 × 7271.0/(T/K)] + 7.84130; temp range –69.3 to 49.7°C (Antoine eq., Weast 1972–73)
　　42585, 42550　　　(interpolated-Antoine equations, Boublik et al. 1984)
　　log (P/kPa) = 5.88698 – 1085.038/(229.817 + t/°C); temp range 15.376–50.53°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
　　log (P/kPa) = 5.87001 – 1080.723/(229.842 + t/°C); temp range 0–45°C (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1984)

42540   (interpolated-Antoine eq., temp range –42 to 73°C, Dean 1985, 1992)

log (P/mmHg) = 6.75483 – 1081.176/(229.34 + t/°C); temp range –42 to 73°C (Antoine eq., Dean 1985, 1992)

42700   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.87963 – 1081.14/(229.349 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

42560   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.87731 – 1079.789/(–43.978 + T/K); temp range 293–324 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 33.1285 – 2.4527×10^3/(T/K) –9.2016·log (T/K) – 4.7077×10^{-10}·(T/K) + 4.1755×10^{-6}·(T/K)^2; temp range 174–489 K (vapor pressure eq., Yaws 1994)

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

173000   (calculated-P/C, Mackay & Shiu 1981)

196800   (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

196800, 49430   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

173180   (calculated-P/C, Eastcott et al. 1988)

188040   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

153890   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.82   (calculated-fragment const., Valvani et al. 1981)

3.25   (calculated-V_M, Wang et al. 1992)

3.82   (recommended, Sangster 1993)

3.82   (Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = (2.66 ± 0.08) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = (2.59 - 6.16) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 297–299 K (Atkinson 1985)

k_{OH}* = (2.22 - 0.36) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 299 K, measured range 245–328 K (relative rate method, Harris & Kerr 1988; Atkinson 1989)

k_{OH}* = 2.32 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k_{OH}* = 2.34 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

2.1.1.1.6   2,3-Dimethylbutane

Common Name: 2,3-Dimethylbutane
Synonym: diisopropyl
Chemical Name: 2,3-dimethylbutane
CAS Registry No: 79-29-8
Molecular Formula: C_6H_{14}; $CH_3CH(CH_3)CH(CH_3)CH_3$
Molecular Weight: 86.175
Melting Point (°C):
    –128.10   (Lide 2003)
Boiling Point (°C):
    57.93   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6616, 0.6570   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
    0.6616   (Weast 1984)
Molar Volume (cm³/mol):
    130.25, 131.16   (20°C, 25°C, calculated-density)
    140.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    29.12, 27.275   (25°C, bp, Dreisbach 1959)
    29.125, 27.276   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    0.812   (Dreisbach 1959)
    0.7991   (Riddick et al. 1986)
    6.43, 2.37, 0.79   (–137.05, –166.15, –127.95°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    52.96, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section.):
    32.9, 22.5   (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
    19.1*   (shake flask-GC, measured range 25–149.5°C, Price 1976)
    11.0   (selected, Riddick et al. 1986)
    21.0*   (IUPAC tentative value, temp range 0 – 150°C, Shaw 1989a)
    18.67*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    28955*   (23.10°C, ebulliometry, measured range: 14.256–58.789°C, Willingham et al. 1945)
    log (P/mmHg) = 6.80983 – 1127.187/(228.900 + t/°C); temp range 14.256–58.789°C (Antoine eq. from exptl.
        data, ebulliometry, Willingham et al. 1945)
    31204*   (calculated-Antoine eq. regression, temp range –63.6 to 58°C, Stull 1947)
    31280   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.90983 – 1127.187/(228.9 + t/°C); temp range –20 to 100°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    31277*   (Antoine eq., temp range –34.9 to 81.3°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.80983 – 1127.187/(228.900 + t/°C); temp range –34.9 to 81.3°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 7120.0/(T/K)] + 7.536008; temp range –63.6 to 225.5°C (Antoine eq., Weast
        1972–73)

31280   (interpolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 5.594371– 1132.099/(229.494 + t/°C); temp range 14.256–58.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

32010   (interpolated-Antoine eq., temp range –35 to 81°C, Dean 1985, 1992)

log (P/mmHg) = 6.80983 – 1127.83/(228.90 + t/°C); temp range –35 to 81°C (Antoine eq., Dean 1985, 1992)

31300   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.93941 – 1129.73/(229.215 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

31290   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.95181 – 1136.355/(–43.159 + T/K); temp range 278–322 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 33.6319 – 2.5524 × 10^3/(T/K) – 9.3142·log (T/K) + 1.4759 × 10^{-10}·(T/K) + 3.914 × 10^{-6}·(T/K)^2; temp range 145–500 K (vapor pressure eq., Yaws 1994)

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

130000   (recommended, Mackay & Shiu 1981)

141000   (calculated-P/C, Mackay & Shiu 1981)

131190   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.85   (shake flask, Hansch & Leo 1979)

3.85   (calculated-fragment const., Valvani et al. 1981)

3.85   (recommended, Sangster 1989, 1993)

2.42; 2.63   (calculated-S, calculated-molar volume, Wang et al. 1992)

3.42   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

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

k$_{OH}$*(exptl) = 5.16 × 10^{12} cm^3 mol^{-1} s^{-1}, k$_{OH}$(correlated) = 4.49 × 10^{12} cm^3 mol^{-1} s^{-1} at 300 K, measured range 300–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k$_{O(3P)}$ = 2.0 × 10^{-13} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom at room temp. (Herron & Huie 1973)

k$_{OH}$ = 5.50 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)

k$_{OH}$ = 5.50 × 10^{-12} cm^3 molecule^{-1} s^{-1}; k$_{O(3P)}$ = 2.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at room temp. (abstraction mechanism, Gaffney & Levine 1979)

k$_{OH}$ = (5.67 ± 0.29) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

k$_{OH}$ = (6.26 ± 0.06) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k$_{NO3}$ = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (relative rate method, Atkinson et al. 1988)

k$_{OH}$* = (5.90 - 0.23) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 K, measured range 247–327 K (relative rate method, Harris & Kerr 1988)

k$_{OH}$ = 6.2 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k$_{OH}$ = 6.3 × 10^{-12} cm^3 molecule^{-1} s^{-1} with an estimated atmospheric lifetime of 22 h in air during summer daylight (Altshuller 1991)

k$_{OH}$ = 6.30 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k$_{NO3}$ = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k$_{OH}$ = 19.0 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k$_{NO3}$ = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

k$_{NO3}$ = (4.04 - 5.34) × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (review, Atkinson 1991)

k$_{OH}$ = 6.3 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, k$_{NO3}$ = 40.6 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

k_{NO3}(exptl) = 4.08×10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO3}(recommended) = 2.55×10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) = 2.55×10^{-16} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 5.78×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 4.40×10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 6.30×10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radicals and an estimated atmospheric lifetime of 22 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.6.1
Reported aqueous solubilities of 2,3-dimethylbutane at various temperatures

Polak & Lu 1973		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		shake flask-GC/FID		IUPAC tentative values		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	32.9	25	19.1	0	33	25	18.67
25	22.5	40.1	19.2	25	21	40.1	18.19
		55.1	23.7	30	19	55.1	20.11
		99.1	40.1	41	19	99.1	39.74
		1213	56.8	50	21	121.3	67.03
		137.3	97.9	70	28	137.3	100.5
		149.5	171	90	35	149.5	138.8
				110	46		
				130	75		
				150	180		
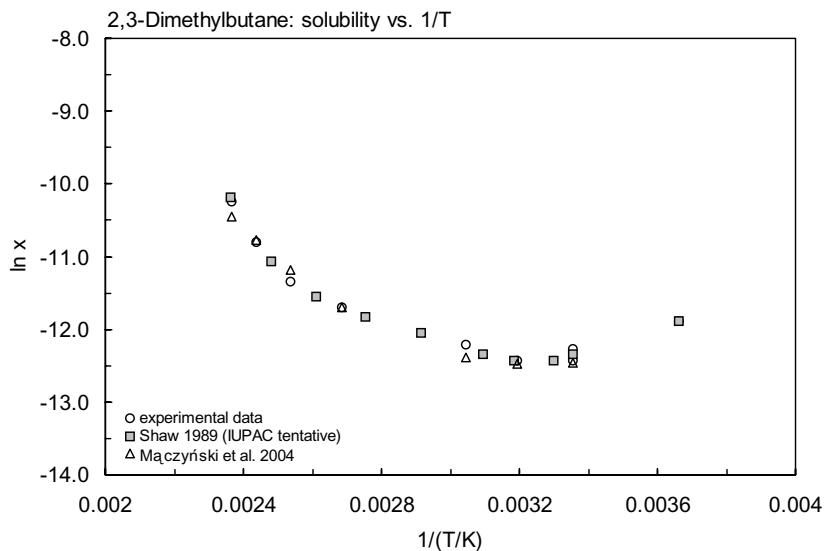
FIGURE 2.1.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2,3-dimethylbutane.

TABLE 2.1.1.1.6.2
Reported vapor pressures of 2,3-dimethylbutane 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)	

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971			
ebulliometry		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
14.256	19921	−63.6	133.3	−34.9	1333	57.988	101325
18.044	23451	−44.5	666.6	−24.3	2666	25.0	234.6
23.099	28955	−34.9	1333	−17.5	4000		
27.746	34897	−24.1	2666	−12.5	5333	eq. 2	P/mmHg
33.357	43320	−12.4	5333	−8.4	6666	A	6.80983
39.15	53654	−4.9	7999	−4.9	7999	B	1127.187
45.339	66756	5.40	13332	0.82	10666	C	228.900
52.06	83718	21.1	26664	5.34	13332		
56.806	97604	39.0	53329	14.36	19998	bp/°C	57.998
57.317	99201	58.0	101325	21.097	26664	ΔH_V/(kJ mol⁻¹) =	
57.79	100693			26.588	33331	at 25°C	29.12
58.32	102390	mp/°C	−128.2	31.257	39997	at bp	27.28
58.789	103907			38.982	53329		
				45.927	66661		
bp/°C	57.988			50.682	79993		
eq. 2	P/mmHg			55.404	93326		
A	6.80983			56.283	95992		
B	1127.187			57.145	98659		
C	228.900			57.568	99992		
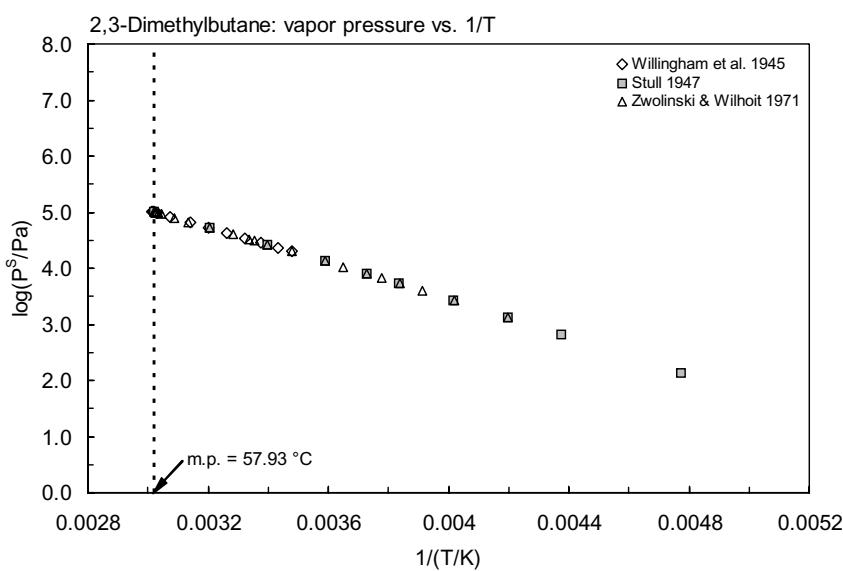
FIGURE 2.1.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylbutane.

2.1.1.1.7   2,2,3-Trimethylbutane

Common Name: 2,2,3-Trimethylbutane
Synonym: triptene
Chemical Name: 2,2,3-trimethylbutane
CAS Registry No: 464-06-2
Molecular Formula: C_7H_{16}; $CH_3CH(CH_3)_2CH(CH_3)_2$
Molecular Weight: 100.202
Melting Point (°C):
    –24.6   (Lide 2003)
Boiling Point (°C):
    80.86   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6901, 0.6859   (20°C, 25°C, Dreisbach 1959)
    0.6901   (Weast 1984)
Molar Volume (cm³/mol):
    145.2, 146.1 (20°C, 25°C, calculated-density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    32.037, 28.94   (25°C, at normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    2.259   (at mp, Dreisbach 1959; Chickos et al. 1999)
    2.36, 2.2   (–152.15, –25.45°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    28.53, 36.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    4.38   (estimated-nomograph of Kabadi & Danner 1979; Brookman et al. 1985)
    7.09   (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    13840   (25.3°C, ebulliometry, measured range 12.6-81.8°C, Forziati et al. 1949)
    log (P/mmHg) = 6.79230 – 1200.563/(226.650 + t/°C); temp range 12.6–81.8°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
    13650   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.79230 – 1200.563/(226.05 + t/°C); temp range 0 – 125°C (Antoine eq. for liquid state, Dreisbach 1959)
    13652   (derived from compiled data, temp range –18.8–205.94°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.79230 – 1200.563/(226.050 + t/°C); temp range –18.8–205.94°C (Antoine eq., Zwolinski & Wilhoit 1971)
    13650, 13660   (interpolated-Antoine equations, Boublik et al. 1984)
    log (P/kPa) = 5.92699 – 11206.087/(226.731 + t/°C); temp range 22.7–105.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    log (P/kPa) = 5.92037 – 1202.337/(226.256 + t/°C); temp range 12.6–81.77°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
    13650   (interpolated-Antoine eq., temp range –19 to 106°C, Dean 1985, 1992)
    log (P/mmHg) = 6.79230 – 1200.563/(226.05 + t/°C); temp range –19 to 106°C (Antoine eq., Dean 1985, 1992)
    13650   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 5.9181 - 1201.098/(-47.026 + T/K)$; temp range 284–355 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/\text{kPa}) = 6.18145 - 1390.726/(-20.97 + T/K)$; temp range 353–483 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/\text{mmHg}) = 32.3633 - 2.6614 \times 10^3/(T/K) - 8.7743 \cdot \log (T/K) - 7.687 \times 10^{-10} \cdot (T/K) + 3.2006 \times 10^{-6} \cdot (T/K)^2$; temp range 249–531 K (vapor pressure eq., Yaws 1994)

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

241010   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH}*(exptl) = 3.84×10^{12} cm³ mol⁻¹ s⁻¹, k_{OH}(correlated) = 3.15×10^{12} cm³ mol⁻¹ s⁻¹ at 296 K, measured range 296–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{OH} = (3.6 - 5.05) × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 296–305 K (Darnall et al. 1978)

k_{OH} = (4.21 ± 0.08) × 10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 5.23×10^{-12} cm³ molecule⁻¹ s⁻¹ at 296 K, k_{OH} = 4.09×10^{-12} cm³ molecule⁻¹ s⁻¹ at 297 K (Atkinson 1985)

k_{OH}* = 4.23×10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990)

k_{NO3}(exptl) = 2.23×10^{-16} cm³ molecule⁻¹ s⁻¹, k_{NO3}(calc) = 1.31×10^{-16} cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 4.24×10^{-12} cm³ molecule⁻¹ s⁻¹, k_{NO3}* = 2.4×10^{-16} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

2.1.1.1.8   n-*Pentane*
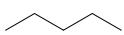
Common Name: *n*-Pentane
Synonym: pentane
Chemical Name: *n*-pentane
CAS Registry No: 109-66-0
Molecular Formula: C_5H_{12}; $CH_3(CH_2)_3CH_3$
Molecular Weight: 72.149
Melting Point (°C):
    –129.67   (Lide 2003)
Boiling Point (°C):
    36.06   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.6262, 0.6214   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    115.22, 116.1   (20° C, 25°C, calculated-density)
    118.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    26.42, 25.77   (25°C bp, Dreisbach 1959)
    26.427, 25.786   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    8.393   (Dreisbach 1959; Riddick et al. 1986)
    8.4   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    58.59, 63.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    360   (16°C, cloud point, Fühner 1924)
    120   (radiotracer method, Black et al. 1948)
    38.5   (shake flask-GC, McAuliffe 1963, 1966)
    49.7   (vapor saturation-GC, Barone et al. 1966)
    40.0   (Baker 1967)
    40.3*   (shake flask-GC, measured range 4 – 30°C, Nelson & De Ligny 1968)
    11.8*   (shake flask-GC, measured range 5 – 35°C, Pierotti & Liabastre 1972)
    65.7; 47.6, 44.6 (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
    39.5*   (shake flask-GC, measured range 25 – 149.5°C, Price 1976)
    39.0   (shake flask-GC, Kryzanowska & Szeliga 1978)
    40.0   (partition coefficient, Rudakov & Lutsyk 1979)
    40.75   (generator column-GC, Tewari et al. 1982a)
    36.9   (calculated-activity coeff. γ and K_{OW}, Tewari 1982b)
    40.6*   (vapor saturation-GC, measured range 15 – 40°C, Jönsson et al. 1982)
    38.9   (shake flask-GC, Coates et al. 1985)
    38.0   (selected, Riddick et al. 1986)
    42.0*   (IUPAC recommended best value, temp range 0 – 90°C, Shaw 1989)
    ln x = –333.59719 + 14358.472/(T/K) + 47.97436·ln (T/K); temp range 290–400 K (eq. derived from literature
        calorimetric and solubility data, Tsonopoulos 1999)
    44.09*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2 – 422.7 K, Mączyński et al. 2004)

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

68213*   (24.828°C, static method, measured range –65 to 25°C, Messerly & Kennedy 1940)
66760*   (24.37°C, ebulliometry, measured range 13.282–36.818°C, Willingham et al. 1945)
log (P/mmHg) = 6.87372 – 1075.816/(233.369 + t/°C); temp range 13.282–36.818°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
71050*   (interpolated-Antoine eq. regression, temp range –76.6 to 36.1°C, Stull 1947)
68330   (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.85221 – 1064.63/(232.0 + t/°C); temp range –35 to 80°C (Antoine eq. for liquid state, Dreisbach 1959)
68368*   (interpolated- Antoine eq., temp range –50.14 to 57.53°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.87632 – 1075.78/(233.205 + t/°C); temp range –50.14 to 57.53°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 6595.1/(T/K)] + 7.489673; temp range –76.6 to 191°C (Antoine eq., Weast 1972–73)
3400*   (–30.86°C, gas saturation, measured range –129.54 to –30.86°C, Carruth & Kobayashi 1973)
57820*   (20.57°C, ebulliometric method, measured range –4.4 to 68.218°C, Osborn & Douslin 1974)
68330   (interpolated-Antoine eq, Boublik et al. 1984)
log (P/kPa) = 6.12545 – 1132.518/(239.074 + t/°C); temp range –65.2 to 24.83°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.96982 – 1060.916/(231.577 + t/°C); temp range 13.28–36.82°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
log (P/kPa) = 5.99028 – 1071.187/(232.766 + t/°C); temp range –4.4 to 68.21°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1974, Boublik et al. 1984)
70915   (interpolated-Antoine eq., temp range –50 to 58°C, Dean 1985. 1992)
log (P/mmHg) = 6.85296 – 1064.84/(233.01 + t/°C); temp range –50 to 58°C (Antoine eq., Dean 1985, 1992)
69810, 68880, 68330 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)
68330   (lit. average, Riddick et al. 1986)
log (P/kPa) = 5.97786 – 1064.84/(232.012 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
68355   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.6922 – 1686.65/(T/K); temp range 143–233 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.99466 – 1073.139/(–40.188 + T/K); temp range 223–352 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.98799 – 1070.14/(–40.485 + T/K); temp range 269–335 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.28417 – 1260.973/(–14.031 + T/K); temp range 350–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.47436 – 2414.137/(141.919 + T/K); temp range 418–470 K (Antoine eq., Stephenson & Malanowski 1987)
68340*   (recommended, Ruzicka & Majer 1994)
ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{2.73425 – 1.988544 × 10^{-3}·(T/K) + 2.408406 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 309.209 K (Cox equation, Ruzicka & Majer 1994)
log (P/mmHg) = 33.3239 – 2.4227 × 10^3/(T/K) – 9.2354·log (T/K) + 9 .0199 × 10^{-11}·(T/K) + 4.105 × 10^{-6}·(T/K)^2; temp range 143–470 K (vapor pressure eq., Yaws 1994)

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

127050   (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
115900, 33430   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
128000   (calculated-P/C, Mackay & Shiu 1975, 1990; Bobra et al. 1979; Mackay et al. 1979; Mackay 1981)
125000   (recommended, Mackay & Shiu 1981)
128000, 125000, 123000, 122200, 10370 (calculated-P/C, Mackay & Shiu 1981)
78050, 99075, 126800, 144020, 174480 (14.8, 20.05, 25.1, 30.1, 34.92°C, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)
121410*   (calculated-temp dependence eq. derived from exptl data, measured range 15–35°C. Jönsson et al. 1982)

ln $(1/K_{AW})$ = 19237.8/(T/K) + 53.671·ln (T/K) – 372.214; temp range: 15 – 35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

127670   (selected, Mills et al. 1982)

120970   (calculated-P/C, Eastcott et al. 1988)

100980   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

128050   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.50   (shake flask-GC, Hansch et al. 1968)

3.39   (shake flask-GC, Leo et al. 1975)

2.99, 3.42, 3.48   (calculated-fragment const., Rekker 1977)

3.23   (Hansch & Leo 1979)

3.64   (calculated-activity coeff. γ, Wasik et al. 1981,1982)

3.62   (generator column-GC, Tewari et al. 1982a,b)

2.37   (HPLC-k′ correlation, Coates et al. 1985)

3.62, 3.60   (generator column-GC, calculated-activity coeff. γ, Schantz & Martire 1987)

3.45   (recommended, Sangster 1989, 1993)

3.39   (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

2.05*   (20.29°C, from GC-determined γ° in octanol, measured range 20.29 – 50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O(3P)}$ = 5.8 × 10^{-14} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) (Herron & Huie 1973)

k_{OH} = (3.74 ± 0.13) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

k_{OH} = 5.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1979)

k_{OH} = 5.0 × 10^{-12} cm^3 molecule^{-1} s^{-1}; $k_{O(3P)}$ = 5.8 × 10^{-14} cm^3 molecule^{-1} s^{-1} room temp. (abstraction mechanism, Gaffney & Levine 1979)

k_{OH} = 4.13 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 299 ± 2 K (relative rate method, Atkinson et al. 1982a)

k_{NO3} = (8.1 ± 1.7) × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (relative rate method, Atkinson et al. 1984a; Atkinson 1991)

k_{OH} = (4.13 ± 0.08) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 4.06 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

k_{OH} = 4.29 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in Smog chamber (Nolting et al. 1988)

k_{OH}* = 3.94 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1991)

k_{OH} = 4.06 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 8.0 × 10^{-17} cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

k_{NO3} = 8.1 × 10^{-17} cm^3 molecule^{-1} s^{-1}, k_{OH} = 3.94 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K with summer daylight atmospheric lifetime τ = 35 h (Altshuller 1991)

k_{OH}* = 3.94 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, k_{NO3} = 9.0 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

k_{NO3}(exptl) = 8.2 × 10^{-17} cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) = 7.7 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 4.00 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 8.7 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

k_{OH}* = 3.70 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 3.94×10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radical and an estimated atmospheric lifetime $\tau = 35$ h (Altshuller 1990).

TABLE 2.1.1.1.8.1
Reported aqueous solubilities of *n*-pentane at various temperatures

1.

Nelson & De Ligny 1968		Pierotti & Liabastre 1972		Polak & Lu 1973		Price 1976	
shake flask-GC		shake flask-GC		shake flask-GC		shake flask-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
4.0	40.9	5.11	10.94	0	65.7	25	39.6
10	42.9	15.21	11.80	25	47.6	40.1	39.8
20	39.3	25.11	11.20			55.7	41.8
25	40.5	35.21	10.89			99.1	69.4
30	40.5					121.3	110
						137.3	210
						149.5	298

2.

Jonsson et al. 1982		Shaw 1989a		Mączyński et al. 2004	
vapor saturation-GC		IUPAC recommended		calc-recommended LLE data	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
15	42.9	0	66	0	56.12
20	41.4	10	43	4	52.11
25	40.6	20	40	10	48.1
30	40.3	25	42	15	48.1
40	40.6	30	41	20	44.09
		40	40	25	44.09
		50	41	30	44.09
		60	43	35.1	44.09
		70	46	40.1	44.09
		80	50	55.7	48.1
		90	58	99.1	88.18
		110	86	121.3	136.3
		130	150	137.3	192.4
		150	300	149.5	260.5
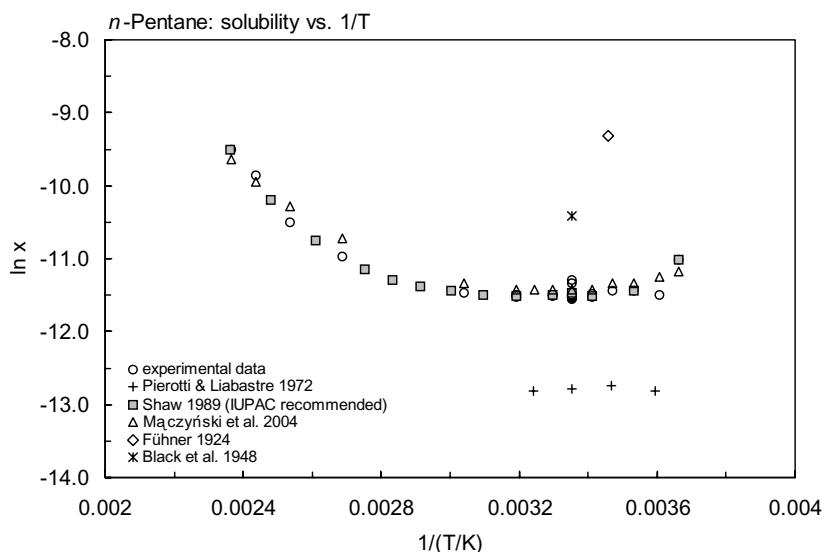
FIGURE 2.1.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *n*-pentane.

TABLE 2.1.1.1.8.2
Reported vapor pressures of *n*-pentane 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)	
log (P/P$_\Phi$) = A[1 − Φ/(T/K)]	(5)	where log A = a + b(T/K) + c(T/K)^2 - Cox eq. I
ln [(P/kPa)/(P$_o$/kPa)] = [1 − (T$_o$/K)/(T/K)]·exp{A$_0$ − A$_1$·(T/K) + A$_2$·(T/K)^2} (6)		- Cox eq. II

1.

Messerly & Kennedy 1940		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static method-manometer		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−65.178	411	13.282	43322	−76.6	133.3	−50.14	1333
−48.811	1604	18.647	53657	−62.5	666.6	−40.25	2666
−39.537	2818	24.371	66756	−50.1	1333	−33.86	4000
−27.420	5951	30.592	83719	−40.1	2666	−29.24	5333
−17.476	10340	34.981	97604	−29.2	5333	−25.42	6666
−9.793	15341	35.453	99201	−22.2	7999	−22.19	7999
−2.359	21933	35.89	100694	−12.6	13332	−16.98	10666
3.618	28767	36.379	102393	1.9	26664	−12.59	13332
9.621	37303	36.818	103911	18.5	53329	−4.33	19998
14.653	45947			36.1	101325	1.92	26664
18.613	53773	bp/°C	36.073			7.01	33331
21.679	60539			mp/°C	−129.7	11.34	39997

(*Continued*)

TABLE 2.1.1.1.8.2 (*Continued*)

Messerly & Kennedy 1940		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static method-manometer		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.828	68213	eq. 2	P/mmHg			18.48	53329
		A	6.87372			24.322	66661
		B	1076.816			29.297	79993
		C	233.359			33.657	93326
						34.469	95992
						35.264	98659
						36.042	101325
						25.0	68368
						bp/°C	36.042
						eq. 2	P/mmHg
						A	6.87632
						B	1075.78
						C	233.205
						$\Delta H_V/(kJ\ mol^{-1}) =$	
						at 25°C	26.43
						at bp	25.77

2.

Carruth & Kobayashi 1973		Osborn & Douslin 1974		Ruzicka & Majer 1994	
gas saturation		ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–129.54	0.0809	–4.40	19933	144.82	0.1
–122.64	0.3893	0.512	25023	157.65	1
–115.87	0.7666	5.464	31177	173.73	10
–108.74	2.6	10.458	38656	193.17	100
–93.55	19.2	15.495	47375	219.13	1000
–83.75	56.93	20.572	57818	255.05	10000
–67.19	285.3	25.698	70121	309.21	101325
–54.18	926.6	30.86	84533	298.15	68350
–45.94	1733	36.068	101325		
–30.86	3400	41.32	120792	data calc from Cox eq.	
		46.613	143245	eq. 6	P/kPa
mp/°C	–129.7	51.951	169019	A_0	2.73425
		57.331	198487	A_1	1.966544×10^{-3}
eq. 1a	P/mmHg	62.755	232016	A_2	2.408406×10^{-6}
A	19.7269	68.218	270022	with reference state at	
B	3899.67			P_o/kPa	101.325
		Cox eq.		T_o/K	309.21
		eq. 5	P/mmHg		
		Φ	309.218		
		a	0.81357		
		b	-7.73685×10^{-4}		
		c	9.06731×10^{-7}		
		P_Φ	760		
		temp range: 268–342 K			

FIGURE 2.1.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-pentane.

TABLE 2.1.1.1.8.3
Reported Henry's law constants and octanol-air partition coefficients of *n*-pentane 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)	

Henry's law constant		log K_{OA}	
Jönsson et al. 1982		Gruber et al. 1997	
equilibrium cell-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
15.0	78035#	20.29	2.053
15.1	77905	30.3	1.911
15.1	77905	40.4	1.781
20.0	98674	50.28	1.670
20	100713#		
20	97490		
25.0	121511		
25	125828		
25	127774		
30.0	146533#		
30	144022		
35.0	173105#		
35	175477		

interpolated from exptl data
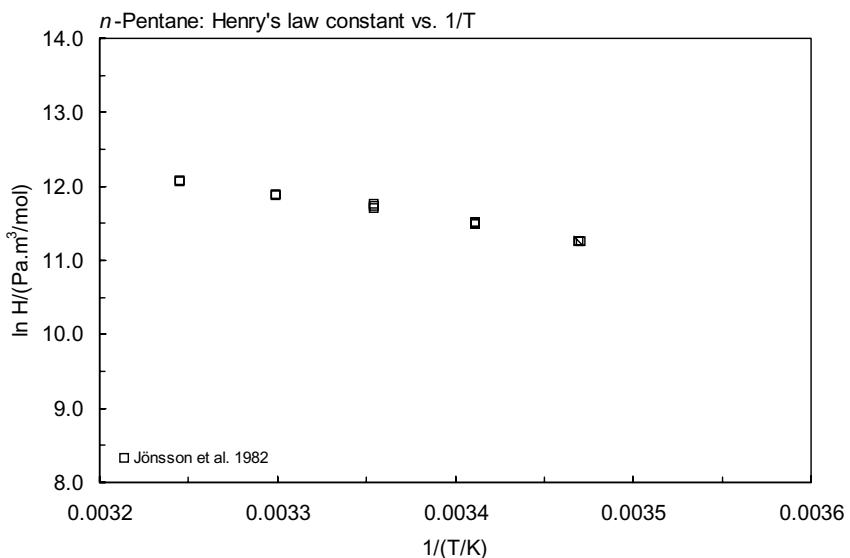
FIGURE 2.1.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-pentane.
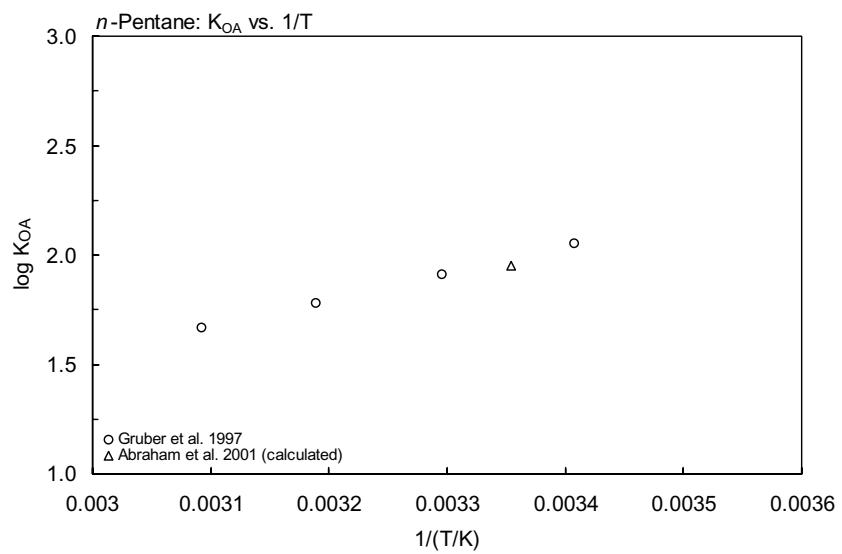
FIGURE 2.1.1.1.8.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-pentane.

2.1.1.1.9   2-Methylpentane (Isohexane)
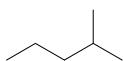
Common Name: 2-Methylpentane
Synonym: isohexane
Chemical Name: 2-methylpentane
CAS Registry No: 107-83-5
Molecular Formula: C_6H_{14}; $CH_3CH(CH_3)CH_2CH_2CH_3$
Molecular Weight: 86.175
Melting Point (°C):
   –153.6   (Lide 2003)
Boiling Point (°C):
   60.26   (Lide 2003)
Density (g/cm³ at 20°C):
   0.6322, 0.6485 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
   136.31, 132.88 (20°C, 25°C, calculated-density)
   140.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   29.87, 27.79 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   6.203   (Dreisbach 1959)
   6.268   (Riddick et al. 1986)
   6.27   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   52.43, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
   compiled at the end of this section.):
   13.8   (shake flask-GC, McAuliffe 1963, 1966)
   16.21   (vapor saturation-GC, Barone et al. 1966)
   19.45; 15.7, 15.6   (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
   14.2   (shake flask-GC, Leinonen & Mackay 1973)
   13.0*   (shake flask-GC, measured range 25 – 149.5°C, Price 1976)
   13.7*   (recommended best value, temp range 25 – 150°C, IUPAC Solubility Data Series, Shaw 1989a)
   13.88*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
   temperatures designated * are compiled at the end of this section.):
   29040*   (25.64°C, ebulliometry, measured temp range 12.758–61.066°C, Willingham et al. 1945)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t/°C); temp range 12.758–61.066°C (Antoine eq. from exptl.
       data, ebulliometry-manometer, Willingham et al. 1945)
   27820*   (calculated-Antoine eq. regression, temp range –60 to 60.3°C, Stull 1947)
   28240   (calculated from determined data, Dreisbach 1959)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t/°C); temp range –15 to 100°C (Antoine eq. for liquid state,
       Dreisbach 1959)
   28238; 28200* (derived from compiled, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t/°C); temp range –32.1 to 83.4°C (Antoine eq., Zwolinski &
       Wilhoit 1971)
   27780   (interpolated-Antoine eq., Weast 1972-73)

log (P/mmHg) = [–0.2185 × 7676.6/(T/K)] + 7.944630; temp range: –60.9 to 60.3°C (Antoine eq., Weast 1972–73)

28240   (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.86839 – 1151.401/(228.477 + t/°C); temp range 12.78 – 61°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

28230   (interpolated-Antoine eq., temp range –32 to 83°C, Dean 1985, 1992)

log (P/mmHg) = 6.83910 – 1135.41/(226.57 + t/°C); temp range –32 to 83°C (Antoine eq., Dean 1985, 1992)

28300   (selected lit., Riddick et al. 1986)

log (P/kPa) = 5.98850 – 1148.74/(228.166 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

28250   (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.97783 – 1142.922/(–45.657 + T/K); temp range 293–335 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 30.7477 – 2.4888 × 10^3/(T/K) –8.2295·log (T/K) – 2.3723 × 10^{-11}·(T/K) + 3.2402 × 10^{-6} · (T/K)^2; temp range 120–498 K (vapor pressure eq., Yaws 1994)

72190   (50°C, vapor-liquid equilibria VLE data, Horstmann et al. 2004)

log (P/kPa) = 5.99313 – 1151.40/(T/K – 44.673); temp range not specified (Antoine eq., Horstmann et al. 2004)

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

170000   (recommended; Mackay & Shiu 1981)

175490   (calculated as 1/K$_{AW}$, C$_W$/C$_A$, reported as exptl., Hine & Mookerjee 1975)

196800, 49430   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

176160   (calculated-P/C, Eastcott et al. 1988)

83590*   (EPICS-GC, measured range 10 – 30°C, Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 2.959 – 957.2/(T/K); temp range 10 – 30°C (EPICS measurements, Ashworth et al. 1988)

176280   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

746   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K$_{AW}$ = 2.470 – 288/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

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

2.85   (calculated-MCI χ, Murray et al. 1975)

3.23   (calculated-molar volume V$_M$, Wang et al. 1992)

3.74   (calculated-fragment constant, Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

Oxidation: 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$_{OH}$(exptl) = (3.2 ± 0.6) × 10^9 M^{-1} s^{-1} at 305 ± 2 K (relative rate method, Lloyd et al. 1976, Darnall et al. 1976)

k$_{OH}$ = (5.68 ± 0.24) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k$_{OH}$ = 5.6 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k$_{OH}$ = 2.34 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, k$_{NO3}$ = 9.7 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

k$_{OH}$ = 5.6 × 10^{-12} cm^3 molecule^{-1} s^{-1}, estimated atmospheric lifetime was 25 h during summer daylight hours (Altshuller 1991)

k$_{NO3}$(exptl) = 1.71 × 10^{-16} cm^3 molecule^{-1} s^{-1}, k$_{NO3}$(calc) = 1.83 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k$_{OH}$ = 5.3 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k$_{NO3}$ = 1.8 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: half-life of 2.4–24 h based on photooxidation rate constant of 3.2×10^{12} cm^3 mol^{-1} s^{-1} for the gas-phase reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric lifetime was estimated to be 25 h during summer daylight, based on photooxidation rate constant of 5.6×10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with hydroxyl radical in air (Altshuller 1991).

TABLE 2.1.1.1.9.1
Reported aqueous solubilities of 2-methylpentane at various temperatures

Polak & Lu 1973		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		shake flask-GC		IUPAC recommended		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
0	19.45	25	13	25	13.7	0	18.19
25	15.7	40.1	13.8	30	13	25	13.88
		55.7	15.7	40	14	40	13.88
		99.1	27.1	50	15	55.7	15.32
		118	44.9	70	17	99.1	30.64
		137.3	86.8	90	23	118	46.92
		149.5	113	110	36	137.3	76.6
				130	68	145.9	110.12
				150	120		

FIGURE 2.1.1.1.9.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-pentane.

TABLE 2.1.1.1.9.2
Reported vapor pressures and Henry's law constants of 2-methylpentane 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)		
$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2)$	(5)		

Vapor pressure						Henry's law constant	
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Ashworth et al. 1988	
ebulliometry		summary of literature data		selected values		EPICS-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
12.758	16620	−60.9	133.3	−32.1	1333	10	70624
16.82	19921	−41.7	666.6	−21.6	2666	15	70320
20.584	23451	−32.1	1333	−14.8	4000	20	89470
25.617	29038	−214	2666	−9.8	5333	25	83593
30.237	34896	−9.7	5333	−5.7	6666	30	85924
35.810	43322	−1.9	7999	−2.2	7999		
41.507	53656	8.1	13332	3.45	10666	ln H = A −B/(T/K)	
47.714	66757	24.1	26664	8.06	13332	H/(atm m³/mol)	
54.388	83718	41.5	53329	16.92	19998	A	2.959
59.099	97605	60.3	101325	23.624	26664	B	957.2
59.607	99204			29.084	33331		
60.074	100694	mp/°C	−154	33.724	39997		
60.602	102394			41.40	53329		
61.066	103913			47.672	66661		
				53.020	79993		
bp/°C	60.271			57.706	93326		
				58.579	95992		
eq. 2	P/mmHg			59.434	98659		
A	6.93910			60.271	101325		
B	1135.410			25.0	28238		
C	226.572						
				eq. 2	P/mmHg		
				A	6.83910		
				B	1135.410		
				C	226.572		
				bp/°C	60.271		
				$\Delta H_V/(kJ\ mol^{-1}) =$			
				at 25°C	29.76		
				at bp	27.79		
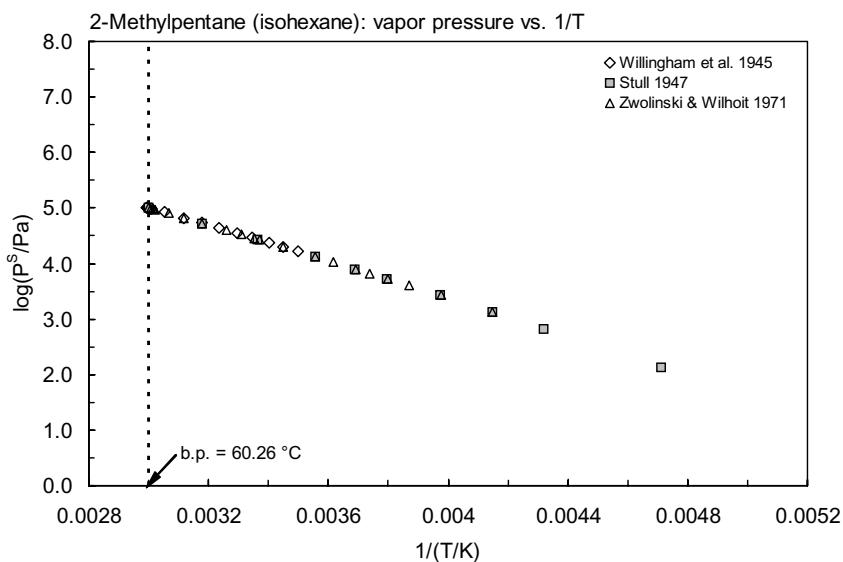
2-Methylpentane (isohexane): vapor pressure vs. 1/T

◇ Willingham et al. 1945
□ Stull 1947
△ Zwolinski & Wilhoit 1971

b.p. = 60.26 °C

FIGURE 2.1.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpentane.

2-Methylpentane (isohexane): Henry's law constant vs. 1/T

□ Ashworth et al. 1988
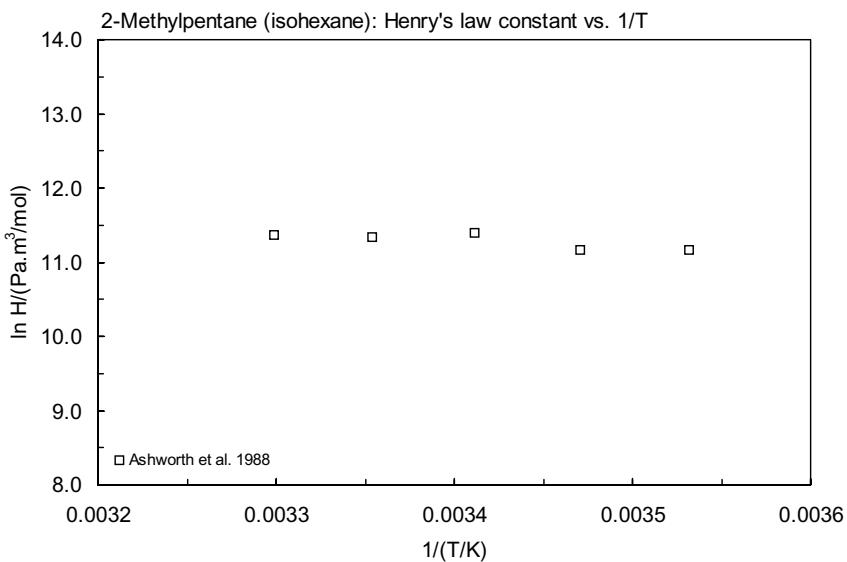
FIGURE 2.1.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylpentane.

2.1.1.1.10   3-Methylpentane
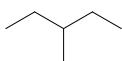
Common Name: 3-Methylpentane
Synonym: diethylmethylmethane
Chemical Name: 3-methylpentane
CAS Registry No: 96-14-0
Molecular Formula: C_6H_{14}; $CH_3CH_2(CH_3)CHCH_2CH_3$
Molecular Weight: 86.175
Melting Point (°C):
    –162.9   (Lide 2003)
Boiling Point (°C):
    63.27   (Lide 2003)
Density (g/cm³ at 25°C):
    0.66431, 0.65976 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    129.7, 130.6 (20°C, 25°C, calculated-density)
    129.7   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
    140.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    30.28, 28.08 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.035   (Riddick et al. 1986)
    5.31   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    48.17, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    12.8   (shake flask-GC, McAuliffe 1966)
    21.5; 17.9, 17.2 (0; 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
    13.1   (shake flask-GC, Price 1976)
    12.9   (partition coefficient-GC, Rudakov & Lutsyk 1979)
    13.0   (selected, Riddick et al. 1986)
    12.9   (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
    22.02, 16.76 (0, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    29040   (23.2°C, ebulliometry, measured range 15.29–64.083°C, Willingham et al. 1945)
    log (P/mmHg) = 6.84887 – 1152.368/(227.129 + t/°C); temp range 15.29–64.083°C (Antoine eq. from exptl.
        data, ebulliometry-manometer, Willingham et al. 1945)
    24970   (Antoine eq. regression, temp range –59 to 63.3°C, Stull 1947)
    25300   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.84887 – 1152.368/(227.129 + t/°C); temp range –15 to 105°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    25305, 25300 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.84887 – 1152.368/(227.129 + t/°C); temp range –30.1 to 86.6°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    24940   (interpolated-Antoine eq., Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 7743.9/(T/K)] + 7.947042; temp range –59 to 63.3°C (Antoine eq., Weast 1972–73)

25310 (interpolated-Antoine eq, Boublik et al. 1984)

log (P/kPa) = 6.36895 − 1997.558/(202.608 + t/°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

25300 (interpolated-Antoine eq., temp range −30 to 87°C, Dean 1985, 1992)

log (P/mmHg) = 6.84887 − 1152.368/(227.13 + t/°C); temp range −30 to 87°C (Antoine eq., Dean 1985, 1992)

25300 (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.98356 − 11133.52/(224.944 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

25320 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.97897 − 1155.28/(−45.659 + T/K); temp range 293–338 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 35.2848 − 2.6773 × 10³/(T/K) − 9.8546·log (T/K) + 2.2352 × 10⁻¹¹·(T/K) + 4.0277 × 10⁻⁶·(T/K)²; temp range 110–504 K (vapor pressure eq., Yaws 1994)

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

172000 (recommended; Mackay & Shiu 1981)

171490 (calculated as 1/K$_{AW}$, C$_W$/C$_A$, reported as exptl., Hine & Mookerjee 1975)

196800, 49430 (calculated-contribution, calculated-bond contribution, Hine & Mookerjee 1975)

170210 (calculated-P/C, Eastcott et al. 1988)

139390 (calculated-MCI χ, Nirmalakhandan & Speece 1988)

113670 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.80 (calculated-π const., Hansch et al. 1968; Hansch & Leo 1979)

2.88 (calculated-MCI χ, Murray et al. 1975)

3.81 (calculated-intrinsic molar volume V$_I$ and solvatochromic parameters, Leahy 1986)

3.60 ± 0.20 (recommended, Sangster 1989)

3.18 (calculated-molar volume V$_M$, Wang et al. 1992)

3.74 (calculated-fragment constant, Müller & Klein 1992)

2.9168 (calculated-UNIFAC group contribution, Chen et al. 1993)

3.60 (recommended, Sangster 1993)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

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

k$_{OH}$ = 1.28 × 10⁹ L mol⁻¹ s⁻¹ at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)

k$_{OH}$ = (4.3 ± 0.9) × 10⁹ M⁻¹ s⁻¹ at 305 ± 2 K (relative rate method, Lloyd et al. 1976)

k$_{OH}$ = 6.82 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at atmospheric pressure and 305 K (Darnall et al. 1978)

k$_{OH}$ = (5.78 ± 0.11) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (relative rate, Atkinson et al. 1984c)

k$_{OH}$ = 5.7 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990, 1991)

k$_{OH}$ = 5.7 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K, estimated atmospheric lifetime 25 h, during summer daylight hours (Altshuller 1991)

k$_{NO3}$(exptl) = 2.04 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹, k$_{NO3}$(calc) = 2.53 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k$_{OH}$ = 5.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, k$_{NO3}$* = 2.2 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 4.30×10^{12} cm^3 mol^{-1} s^{-1} with hydroxyl radical with half-life of 2.4–24 h (Darnall et al. 1976; Lloyd et al. 1976);

rate constant of 5.7×10^{-12} cm^3 molecule$^{-1} \cdot$s^{-1} for the reaction with OH radical with an estimated atmospheric lifetime of 25 h during summer daylight (Altshuller 1991).

2.1.1.1.11   2,2-Dimethylpentane
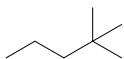
Common Name: 2,2-Dimethylpentane
Synonym:
Chemical Name: 2,2-dimethylpentane
CAS Registry No: 590-35-2
Molecular Formula: C_7H_{16}; $CH_3C(CH_3)_2CH_2CH_2CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –123.7   (Lide 2003)
Boiling Point (°C):
    79.2   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6739   (Weast 1984)
    0.6739, 0.6695   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    148.69   (20°C, calculated from density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.812   (Dreisbach 1959)
    5.86   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    39.55, 49.74 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    4.40   (shake flask-GC, Price 1976)
    4.90   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    13824   (24.67°C, manometer, measured range 15.325–80.05°C, Willingham et al. 1945)
    log (P/mmHg) = 6.81509 – 1190.298/(223.343 + t/°C); temp range 15.325–80.05°C (Antoine eq. from exptl. data, ebulliometry-manometer measurements, Willingham et al. 1945)
    13850   (24.708°C, ebulliometry, Forziati et al. 1949)
    log (P/mmHg) = 6.81479 – 1190.033/(223.303 + t/°C); temp range 12.188–80.074°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
    14030   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.81480 – 1190.033/(223.303 + t/°C); temp range 0–115°C (Antoine eq. for liquid state, Dreisbach 1959)
    14026   (interpolated-Antoine eq., temp range –18.6 to 103.75°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.81480 – 1190.033/(223.303 + t/°C); temp range –18.6 to 103.75°C (Antoine eq., Zwolinski & Wilhoit 1971)
    13500   (interpolated-Antoine eq., temp range –69.3 to 49.7°C, Weast 1972–72)
    log (P/mmHg) = [–0.2185 × 7271.0/(T/K)] + 7.841340; temp range –69.3 to 49.7°C (Antoine eq., Weast 1972–73)
    14030   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.93788 – 1189.09/(223.198 + t/°C); temp range 15.32-80.05°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
    14030   (interpolated-Antoine eq., temp range –18 to 103°C, Dean 1985, 1992)
    log (P/mmHg) = 6.84180 – 1190.033/(223.3 + t/°C); temp range –18 to 103°C (Antoine eq., Dean 1985, 1992)
    14010   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.93117 - 1185.576/(-50.37 + T/K)$; temp range 277-354 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.2280 - 1399.333/(-20.934 + T/K)$; temp range 353–483 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/mmHg) = 6.2875 - 2.1682 \times 10^3/(T/K) + 2.6936 \cdot log (T/K) - 1.5525 \times 10^{-2} \cdot (T/K) + 1.0917 \times 10^{-5} \cdot (T/K)^2$; temp range 149–527 K (vapor pressure eq., Yaws 1994)

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

318000   (calculated-P/C, Mackay & Shiu 1981)
319200   (selected, Mills et al. 1982)
319420   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.10   (calculated-π substituent constant, Hansch et al. 1968)
3.62   (calculated-V_M, Wang et al. 1992)
4.14   (calculated-fragment constant, Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures see reference:
   $k_{OH} = (2.66 \pm 0.08) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)
   $k_{OH} = 3.37 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (Atkinson 1989)
   $k_{OH} = 3.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)
   $k_{OH} = 2.34 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, $k_{NO3} = 9.7 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)
   $k_{OH} = 3.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.1.12   2,4-Dimethylpentane
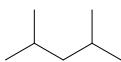
Common Name: 2,4-Dimethylpentane
Synonym: diisopropylmethane
Chemical Name: 2,4-dimethylpentane
CAS Registry No: 108-08-7
Molecular Formula: C_7H_{16}; $CH_3CH(CH_3)CH_2CH(CH_3)CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –119.5   (Lide 2003)
Boiling Point (°C):
    80.49   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6727, 0.6683   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    148.95, 149.9   (20°C, 25°C, calculated-density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    32.89, 29.501   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.840   (Dreisbach 1959)
    6.845   (Riddick et al. 1986)
    6.85   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    44.46, 44.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    3.62   (shake flask-GC, McAuliffe 1963)
    4.06   (shake flask-GC, McAuliffe 1966; quoted, Hermann 1972; Price 1976)
    6.50; 5.50   (0; 25°C, shake flask-GC, Polak & Lu 1973)
    4.41   (shake flask-GC, Price 1976)
    4.20   (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
    6.12, 4.45   (0, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    12635   (Antoine eq. regression, temp range –48 to 80.5°C, Stull 1947)
    11730   (22.54°C, ebulliometry, measured range 13.714–81.374°C, Forziati et al. 1949)
    log (P/mmHg) = 6.82621 –1192.041/(221.634 + t/°C); temp range 13.714–81.374°C (Antoine eq. from exptl. data, ebulliometry-manometer, Forziati et al. 1949)
    13120   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.82621 – 1192.041/(221.634 + t/°C); temp range 0 – 115°C (Antoine eq. for liquid state, Dreisbach 1959)
    13119   (interpolated-Antoine eq, temp range –17.0 to 104.94°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.82621 – 1192.041/(221.634 + t/°C); temp range –17.0 to 104.94°C (Antoine eq., Zwolinski & Wilhoit 1971)
    12620   (interpolated-Antoine eq., temp range –48.0 to 80.5°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 8167.4/(T/K)] + 7.961374; temp range –48.0 to 80.5°C (Antoine eq., Weast 1972–73)
    13120   (interpolated-Antoine eq., temp range 13.7–81.37°C, Boublik et al. 1984)
    log (P/kPa) = 5.95675 – 1195.154/(221.992 + t/°C); temp range 13.7–81.37°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15450 (interpolated-Antoine eq., temp range –17 to 105°C, Dean 1985, 1992)

$\log (P/mmHg) = 6.82621 – 1192.04/(225.32 + t/°C)$; temp range –17 to 105°C (Antoine eq., Dean 1985, 1992)

13000 (selected, Riddick et al. 1986)

$\log (P/kPa) = 5.94917 – 1191.06/(221.540 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

13125 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.95921 – 1196.516/(–50.993 + T/K)$; temp range 284–355 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 35.9436 – 2.846 \times 10^3/(T/K) – 9.9938 \cdot \log (T/K) + 8.0613 \times 10^{-11} \cdot (T/K) + 3.6419 \times 10^{-6} \cdot (T/K)^2$; temp range 154–520 K (vapor pressure eq., Yaws 1994)

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

319300 (calculated–$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

326600, 73120 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

300000 (recommended; Mackay & Shiu 1981)

297300 (calculated-P/C, Eastcott et al. 1988)

160050 (calculated-molecular connectivity index MCI χ, Nirmalakhandan & Speece 1988)

298050 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

3.17 (calculated-MCI χ, Murray et al. 1975)

3.66 (calculated-molar volume V_M, Wang et al. 1992)

4.14 (calculated-f constant, Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

Oxidation: 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:

$k_{OH} = (5.26 \pm 0.11) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 5.10 \times 10^{-12}$ cm^3 · molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k_{NO3}(exptl) $= 1.44 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) $= 2.89 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 $\pm$ 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH} = 5.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}* $= 1.5 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 5.10×10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radicals and an estimated lifetime of 27 h during summer daylight (Altshuller 1991).

2.1.1.1.13   3,3-Dimethylpentane

Common Name: 3,3-Dimethylpentane
Synonym:
Chemical Name: 3,3-dimethylpentane
CAS Registry No: 562-49-2
Molecular Formula: C_7H_{16}; $CH_3CH_2(CH_3)_2CH_2CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –134.4   (Lide 2003)
Boiling Point (°C):
    86.06   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6933, 0.6891   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    144.5   (20°C, calculated-density, Stephenson & Malanowski 1987)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    33.02, 29.74   (25°C, normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.067   (Dreisbach 1959)
    7.07   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    51.16, 49.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end
    of this section.):
    5.94*   (shake flask-GC, measured range 25–150.4°C, Price 1976)
    6.68*   (calculated-liquid-liquid equilibrium LLE data, temp range 298.2–423.2 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    10600*   (Antoine eq. regression, temp range –45.9 to 86.1°C Stull 1947)
    10316*   (23.521°C, ebulliometry, measured range –13.5 to 82°C Forziati et al. 1949)
    log (P/mmHg) = 6.82668 – 1228.063/(225.316 + t/°C); temp range 13.484–80.962°C (Antoine eq., ebulliometry-
        manometer measurements, Forziati et al. 1949)
    11044   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.82667 – 1228.663/(225.316 + t/°C); temp range 5–130°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    11039*   (interpolated-Antoine eq., temp range –14.4 to 111.25°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.82667 – 1228.663/(225.316 + t/°C); temp range –14.4 to 111.25°C (Antoine eq., Zwolinski
        & Wilhoit 1971)
    10600   (interpolated-Antoine eq., temp range –45.9 to 86.1°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 8145.4/(T/K)] + 7.869254; temp range –45.9 to 86.1°C (Antoine eq., Weast
        1972–73)
    11045   (interpolated-Antoine eq., temp range 13.484–86.96°C, Boublik et al. 1984)
    log (P/kPa) = 5.95327 – 1229.625/(225.427 + t/°C); temp range 13.484–86.96°C (Antoine eq. from reported
        exptl. data, Boublik et al. 1984)
    11045   (interpolated-Antoine eq., temp range –14 to 112°C, Dean 1985, 1992)

log (P/mmHg) = 6.82667 – 1228.663/(225.32 + t/°C); temp range –14 to 112°C (Antoine eq., Dean 1985, 1992)

11150, 11040 (interpolated-Antoine eq.-I, III, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.95139 – 1228.138/(–47.819 + T/K); temp range 285–360 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.35011 – 1415.316/(–31.302 + T/K); temp range 213–281 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.94685 – 1225.973/(–48.144 + T/K); temp range 280–360 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 30.2570 – 2.6313 × 10^3/(T/K) – 7.9839·log (T/K) + 4.6848 × 10^{-13}·(T/K) + 2.717 × 10^{-6}· (T/K)^2; temp range 139–536 K (vapor pressure eq., Yaws 1994)

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

186000   (calculated-P/C, Mackay & Shiu 1981)

186305   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

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

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

Half-Lives in the Environment:

TABLE 2.1.1.1.13.1
Reported aqueous solubilities of 3,3-dimethylpentane at various temperatures

Price 1976		Mączyński et al. 2004	
shake flask-GC		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
25	5.92	25	6.68
40.1	6.78	40	6.68
55.7	8.17	56	7.79
69.7	10.3	70	8.91
99.1	15.8	99	16.14
118	27.3	118	26.17
140.4	67.3	150	66.81
150.4	86.1		

FIGURE 2.1.1.1.13.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 3,3-dimethyl-pentane.

TABLE 2.1.1.1.13.2
Reported vapor pressures of 3,3-dimethylpentane 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)		
$\ln (P/P_{ref}) = [1 - (T_{ref}/T)]·\exp(a + bT + cT^2)$	(5)		

Stull 1947		Forziati et al. 1949				Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		set 1		set 2			
–45.9	133.3	13.443	6383	17.163	7658	–14.41	1333
–25.0	666.6	17.231	7677	20.484	8969	–2.96	2666
–14.4	1333	30.533	8985	34.355	16623	4.36	4000
–2.90	2666	23.521	10316	38.804	19926	9.852	5333
9.90	5333	26.318	11704	53.385	34902	14.297	6666
18.1	7999	30.086	13826	59.444	43327	18.055	7999
29.3	13332	34.406	16613	84.792	976–7	24.231	10666
46.2	26664	38.790	19917	85.344	99201	29.241	13332
65.5	53329	48.72	23438	85.854	100696	38.880	19998
86.1	101325	48.34	28954	86.429	102396	46.173	26664
		53.37	34893			52.114	33331
mp/°C	–135	59.44	43322			57.164	39997
		65.697	53645			65.519	53329
		72.384	66733			72.347	66661
		79.651	83682			78.168	79993
		84.78	97575	bp/°C	86.069	83.272	93326
		85.335	99206			84.222	95992

(Continued)

TABLE 2.1.1.1.13.2 (*Continued*)

Stull 1947		Forziati et al. 1949				Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		86.421	102377	eq. 2	P/mmHg	85.153	98659
		86.928	103895	A	6.81813	86.064	101325
				B	1223.543	25.0	11039
				C	224.687		
						eq. 2	P/mmHg
						A	6.82667
						B	1228.663
						C	225.316
						bp/°C	86.064
						ΔH_v/(kJ mol^{-1}) =	
						at 25°C	33.02
						at bp	29.65
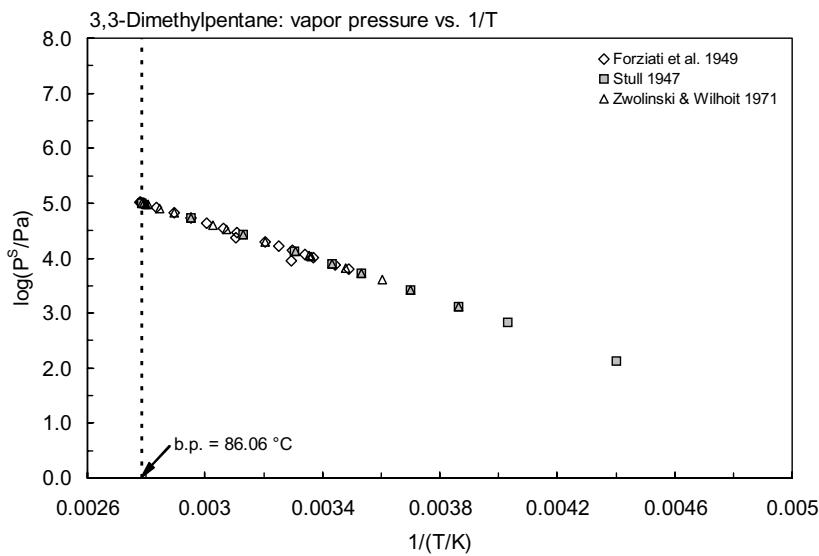
FIGURE 2.1.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 3,3-dimethylpentane.

2.1.1.1.14   2,2,4-Trimethylpentane (Isooctane)
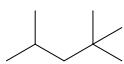
Common Name: 2,2,4-Trimethylpentane
Synonym: isooctane, isobutyltrimethylmethane
Chemical Name: 2,2,4-trimethylpentane
CAS Registry No: 504-84-1
Molecular Formula: C_8H_{18}; $CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$
Molecular Weight: 114.229
Melting Point (°C):
    –107.30   (Stull 1947; Lide 2003)
Boiling Point (°C):
    99.22   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.6919, 0.6878   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    165.1   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
    185.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    36.92, 32.01   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.196   (Riddick et al. 1986)
    9.27   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    55.52, 43.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    2.44   (shake flask-GC, McAuliffe 1963,1966)
    2.46; 2.05   (0; 25°C, shake flask-GC, Polak & Lu 1973)
    1.14   (shake flask-GC, Price 1976)
    2.50, 2.0, 2.20   (0, 20, 25°C, IUPAC recommended values, Shaw 1989b)
    2.30, 1.65, 1.65   (0. 20, 25°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    6371   (24.4°C, ebulliometry, measured temp range 24.4–100.13°C, Willingham et al. 1945)
    log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t/°C); temp range 24.4–100.13°C (Antoine eq., ebulliometry-
        manometer measurements, Willingham et al. 1945)
    6250   (calculated-Antoine eq. regression, temp range –36.4 to 99°C, Stull 1947)
    1739, 6573, 19528   (0, 25, 50°C, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)
    6580   (calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)
    log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t/°C); temp range 15 – 120°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    6573   (interpolated-Antoine eq., temp range –4.3 to 125.22°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t/°C); temp range –4.3 to 125.22°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    6570   (interpolated-Antoine eq., temp range 24.6–100.13°C, Boublik et al. 1973, 1984)
    log (P/mmHg) = 6.80304 – 1252.59/(220.119 + t/°C), temp range 24.6–100.13°C (Antoine eq. from reported
        exptl. data of Willingham et al. 1945, Boublik et al. 1984)
    6240   (interpolated-Antoine eq., temp range –36.5 to 99.2°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 8548.0/(T/K)] + 7.934852; temp range –36.5 to 99.2°C (Antoine eq., Weast
        1972–73)

log (P/kPa) = 5.92751 – 1252.348/(220.09 + t/°C); temp range 69.2 – 271.1°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

6580   (interpolated-Antoine eq., temp range: 24 – 100°C, Dean 1985, 1992)

log (P/mmHg) = 6.81189 – 1257.84/(220.74 + t/°C), temp range: 24 – 100°C (Antoine eq., Dean 1985, 1992)

6500   (quoted lit., Riddick et al. 1986)

log (P/kPa) = 5.92885 – 1153.36/(220.241 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

6580   (interpolated, Antoine eq., Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 5.93934 – 1254.146/(–52.831 + T/K), temp range: 297–314 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 6.44016 – 1650.17/(T/K); temp range 423–523 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 6.33252 – 1441.485/(–36.695 + T/K); temp range 194–299 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 6.97534 – 1283/067/(–40.166 + T/K); temp range 372–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 6.26002 – 1501.036/(–19.15 + T/K); temp range 413–494 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P_L$/kPa) = 7.76427 – 3268.783/(206.659 + T/K); temp range 490–544 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P/mmHg) = 35.954 – 3.0569 × 10^3/(T/K) – 9.8896·log (T/K) – 7.2916 × 10^{-11}·(T/K) + 3.1060 × 10^{-6}·(T/K)^2; temp range 161–564 K (vapor pressure eq., Yaws 1994)

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

308030   (calculated-P/C, Mackay & Leinonen 1975)

330000; 308000, 365000 (recommended; calculated-P/C, Mackay & Shiu 1981)

304960   (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

472090, 110700 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

314110   (calculated-P/C, Lyman et al. 1982)

350140   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

327200   (calculated-P/C, Eastcott et al. 1988)

338270   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

5.83   (estimated-HPLC/MS, Burkhard et al. 1985)

4.54   (calculated-fragment const., Burkhard et al. 1985)

5.02   (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.06   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization: volatilization $t_{1/2}$ = 5.5 h from a water column 1 m^2 in cross section of depth 1 m (Mackay & Leinonen 1975);

$t_{1/2}$ ~ 3.1 h at 20°C in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982).

Photolysis:

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

k_{OH}*(exptl) = 2.83 × 10^{12} cm^3 mol^{-1} s^{-1}, k_{OH}(calc) = 2.35 × 10^{12} cm^3 mole^{-1} s^{-1} at 298 K, measured range 298–493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{OH} = 3.73 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Darnall et al. 1978)

$k_{O(3P)} = 9.10 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom at room temp. (Herron & Huie 1973)

$k_{OH} = 3.7 \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)

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

$k_{OH} = (3.66 \pm 0.16) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 3.90 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K and 3.56×10^{-12} cm^3 molecule^{-1} s^{-1} at 297 K (Atkinson 1985)

$k_{OH} = 3.68 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k_{NO3}(exptl) $= 7.5 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) $= 1.65 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}* = 3.57 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 9.0 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 16 h, based on the photooxidation reaction rate constant of 3.68×10^{-12} cm^3 molecule^{-1} s^{-1} with OH radical in air during summer daylight (Altshuller 1991).

Surface water: volatilization $t_{1/2} = 5.5$ h from a water column 1 m^2 in cross section of depth 1-m (Mackay & Leinonen 1975);

estimated $t_{1/2} = 3.1$ h at 20°C in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m s^{-1} (Lyman et al. 1982).

2.1.1.1.15   2,3,4-Trimethylpentane
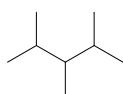
Common Name: 2,3,4-Trimethylpentane
Synonym:
Chemical Name: 2,3,4-trimethylpentane
CAS Registry No: 565-75-3
Molecular Formula: C_8H_{18}; $CH_3CH(CH_3)CH(CH_3)CH(CH_3)CH_3$
Molecular Weight: 114.229
Melting Point (°C):
   –109.2   (Lide 2003)
Boiling Point (°C):
   113.5   (Lide 2003)
Density (g/cm³ at 20°C):
   0.7191   (Weast 1984)
   0.7191, 0.7191   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
   158.9   (calculated-density, Stephenson & Malanowski 1987)
   185.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   38.0, 32.67 (25°C, at normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   9.27   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   56.65, 38.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   2.34, 2.30   (0; 25°C, shake flask-GC, Polak & Lu 1973)
   1.36   (shake flask-GC, Price 1976)
   2.30, 1.36   (quoted lit., IUPAC Solubility Data Series, Shaw 1989)
   2.86, 2.03   (0, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   log (P/mmHg) = 6.85396 – 1315.034/(217.526 + t/°C); temp range 36.568–114.381°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
   3431   (Antoine eq. regression, temp range –26 to 113.5°C Stull 1947)
   3600   (calculated from determined data, Dreisbach 1959)
   log (P/mmHg) = 6.85396 – 1315.084/(217.526 + t/°C); temp range 25 – 150°C (Antoine eq. for liquid state, Dreisbach 1959)
   3600   (interpolated-Antoine eq., temp range 7.1–140.0°C, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.85396 – 1315.084/(217.526 + t/°C); temp range 7.1–140.0°C (Antoine eq., Zwolinski & Wilhoit 1971)
   3430   (interpolated-Antoine eq., temp range –26.3 to 113.5°C, Weast 1972–73)
   log (P/mmHg) = [–0.2185 × 8988.2/(T/K)] + 7.997094; temp range –26.3 to 113.5°C (Antoine eq., Weast 1972–73)
   1179   (4.912°C, static method-inclined piston manometer, measured range –50.325 to 4.912°C, Osborn & Douslin 1974)
   3600   (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.98137 – 1316.608/(217.70 + t/°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

3600   (extrapolated-Antoine eq., temp range 36–114°C, Dean 1985, 1992)

log (P/mmHg) = 6.85396 – 1315.08/(217.53 + t/°C); temp range 36–114°C (Antoine eq., Dean 1985, 1992)

3610   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.00347 – 1330.047/(–53.921 + T/K); temp range 288–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.37038 – 1511.86/(–38.054 + T/K); temp range 223–289 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 35.1565 – 3.0232 × 10^3/(T/K) –9.2267·log (T/K) + 2.7691 × 10^{-11}·(T/K) + 2.7828 × 10^{-6}·(T/K)^2; temp range 164–566 K (vapor pressure eq., Yaws 1994)

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

190000; 302000, 179000   (recommended; calculated-P/C, Mackay & Shiu 1981)

178700   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

     k_{OH}* = 6.99 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 K, measured range 243–313 K (relative rate method with reference to *n*-hexane, Harris & Kerr 1988; Atkinson 1989)

     k_{OH} = 7.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1990)

     k_{OH} = 7.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K and the atmospheric lifetime was estimated to be 20 h during summer daylight hours (Altshuller 1991)

     k_{OH} = 7.1 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 20 h, based on the photooxidation reaction rate constant of 7.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} with OH radicals in air during summer daylight (Altshuller 1991).

2.1.1.1.16   n-*Hexane*
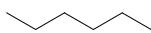
Common Name: *n*-Hexane
Synonym: hexane
Chemical Name: *n*-hexane
CAS Registry No: 110-54-3
Molecular Formula: C_6H_{14}; $CH_3(CH_2)_4CH_3$
Molecular Weight: 86.175
Melting Point (°C):
     –95.35   (Lide 2003)
Boiling Point (°C):
     68.73   (Lide 2003)
Density (g/cm³ at 20°C):
     0.6593, 0.6548   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
     130.7; 131.6 (20°C, 25°C, calculated-density)
     140.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     31.552, 28.853   (25°C, bp, Riddick et al. 1986)
     31.52   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     13.028   (Dreisbach 1959)
     13.079   (Riddick et al. 1986)
     13.08   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     73.22, 72.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

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

     140   (15.5°C, shake flask-cloud point, Fühner 1924)
     < 262   (shake flask-residue volume, Booth & Everson 1948)
     36.0   (shake flask-cloud point, Durand 1948)
     120   (shake flask-cloud point, McBain & Lissant 1951)
     9.50   (shake flask-GC, McAuliffe 1963, 1966;)
     16.2   (vapor saturation-GC, Barone et al. 1966)
     18.3*   (shake flask-GC, measured range 4–55°C, Nelson & De Ligny 1968)
     12.3   (shake flask-GC, Leinonen & Mackay 1973)
     12.4*   (shake flask-GC, Polak & Lu 1973)
     13.0   (shake flask-GC, Krasnoshchekova & Gubertritis 1973)
     16.2   (shake flask-GC, Mackay et al. 1975)
     9.47*   (shake flask-GC, measured range 25–151.8°C, Price 1976)
     12.3   (shake flask-GC, Aquan-Yuen et al. 1979)
     10.09*   (vapor saturation-GC, measured range 15.5–40°C, Jönsson et al. 1982)
     12.24   (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982; Miller et al. 1985)
     14.1   (calculated-activity coeff. γ and K_{OW}, Tewari et al. 1982b)
     11.4*   (37.78°C, shake flask-GC, measured 37.78–200°C, Tsonopoulos & Wilson 1983)
     9.55   (shake flask-GC, Coates et al. 1985)
     14.0   (shake flask-purge and trap-GC, Coutant & Keigley 1988)
     9.8*   (recommended best value, IUPAC Solubility Data Series, temp range 0–140°C, Shaw 1989)
     ln x = –374.90804 + 16327.128/(T/K) + 53.89582·ln (T/K); temp range 290–400 K (eq. derived from literature
          calorimetric and solubility data, Tsonopoulos 1999)
     11.5*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–425 K, Mączyński et al. 2004)

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

24811*   (30°C, static-manometer, measured range 30–60°C, Smyth & Engel 1929)

19920*   (24.7°C, ebulliometry, measured range 13.033–69.541°C Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.87776 - 1171.530/(224.366 + t/°C)$; temp range 13.033–69.541°C (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)

19700*   (calculated-Antoine eq. regression, temp range –53.9 to 68.7°C, Stull 1947)

20170   (calculated from determined data, Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.87776 - 1171.53/(224.366 + t/°C)$; temp range –10 to 110°C (Antoine eq. for liquid state, Dreisbach 1959)

20198*   (interpolated-Antoine eq., temp range –25.1 to 92.1°C, Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.87776 - 1171.530/(224.366 + t/°C)$; temp range –25.1 to 92.1°C (Antoine eq., Zwolinski & Wilhoit 1971)

3120*   (–0.51°C, gas saturation, measured range –95.44 to –0.51°C, Carruth & Kobayashi 1973)

20130   (Campbell et al. 1968)

20124, 20141   (static method-differential pressure gauge, Bissell & Williamson 1975)

22090*   (27.1°C, Letcher & Marsicano 1974)

21809, 57929, 130189 (26.85, 51.85, 76.85°C, vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)

20160   (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.01098 - 1176.102/(224.899 + t/°C)$; temp range 13.033–69.54°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.72763 - 1031.938/(208.304 + t/°C)$; temp range 27.11–45.11°C (Antoine eq. from reported exptl. data of Letcher & Marsicano 1974, Boublik et al. 1984)

20190   (interpolated-Antoine eq., temp range –25 to 92°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.87601 - 1171.17/(224.41 + t/°C)$; temp range –25 to 92°C (Antoine eq., Dean 1985, 1992)

20700, 20180, 20160 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)

20170   (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.00091 - 1171.91/(224.408 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

20180, 20300, 20165   (interpolated-Antoine equations I, II and IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.00431 - 1172.04/(-48.747 + T/K)$; temp range 293–343 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15142 - 1224.492/(-45.358 + T/K)$; temp range 238–298 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.47892 - 1800.89/(-4.115 + T/K)$; temp range 189–259 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99521 - 1167.388/(-49.272 + T/K)$; temp range 298–341 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.91942 - 1123.687/(-54.776 + T/K)$; temp range 341–377 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.4106 - 1469.286/(-7.702 + T/K)$; temp range 374–451 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.30814 - 2367.155/(111.016 + T/K)$; temp range 445–508 K (Antoine eq.-VII, Stephenson & Malanowski 1987)

10854   (calculated-UNIFAC activity coeff., Banerjee et al. 1990)

20136*   (24.96°C, Hg manometer, measured range 9.95–49.97°C, Gracia et al. 1992)

20180*   (recommended, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{2.79797 - 2.022083 \times 10^{-3} \cdot (T/K) + 2.287564 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 341.863$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 69.7378 - 3.6278 \times 10^3/(T/K) - 23.927 \cdot \log (T/K) + 1.281 \times 10^{-2} \cdot (T/K) - 1.6844 \times 10^{-13} \cdot (T/K)^2$; temp range 178–507 K (vapor pressure eq., Yaws 1994)

24938, 53982   (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

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.):

183690   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

160000, 50590   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

190000   (calculated-P/C, Mackay & Shiu 1975,1981; Bobra et al. 1979)

177060   (equilibrium cell-concn ratio-GC, Vejrosta et al. 1982)

173340*   (equilibrium cell-concentration ratio-GC, measured range 14.52–34.9°C Jönsson et al. 1982)

103262, 135400, 172140, 215420, 261420   (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)

$\ln (1/K_{AW}) = 21493.1/(T/K) + 59.299 \cdot \ln (T/K) - 414.193$; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

77820*   (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln [H/(atm\_m^3/mol)] = 25.25 - 7530/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

130790   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

18600*   (40°C, equilibrium headspace-GC, measured range 40–70°C, Kolb et al. 1992)

$\ln (1/K_{AW}) = -28.60 + 8375/(T/K)$; temp range 40–70°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

163812   (EPICS-GC, Ryu & Park 1999)

65318   (20°C, selected from reported experimental values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 12.150 - 3143/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

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

3.00   (calculated-π constant, Hansch et al. 1968; Hansch & Leo 1979)

3.90   (shake flask-concn. ratio-GC, Platford 1979; Platford 1983)

4.20   (calculated-activity coeff. γ, Wasik et al. 1981, 1982)

4.11   (generator column-GC, Tewari et al. 1982a,b)

2.90   (HPLC-k′ correlation, Coates et al. 1985)

4 25   (calculated-activity coeff., Berti et al. 1986)

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

4.00   (recommended, Sangster 1989, 1993)

4.29   (calculated-activity coeff., Tse & Sandler 1994)

3.90   (recommended, Hansch et al. 1995)

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

2.55*   (20.29°C, from GC-determined γ° in octanol, measured range 20.29–50.28°C Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O(3P)} = 9.30 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atoms (Herron & Huie 1973)

$k_{OH} = (3.8 \pm 0.8) \times 10^9$ L mol^{-1} s^{-1} at 305 K (relative rate method, Llyod et al. 1976)

$k_{OH} = 5.90 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)

$k_{OH} = (6.1 - 6.8) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} 292–303 K, k_{OH} (calc) = 6.96×10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (Darnall et al. 1978)

$k_{OH} = 5.90 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}; $k_{O(3P)} = 9.3 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atoms, at room temp. (abstraction mechanism, Gaffney & Levine 1979)

$k_{OH} = (5.71 \pm 0.09) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 299 ± 2 K (relative rate method, Atkinson et al. 1982a)

$k_{NO3} = (1.05 \pm 0.2) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson et al. 1984a, Atkinson 1991)

$k_{OH} = (5.70 \pm 0.09) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 5.21 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson & Aschmann 1984)

k_{OH} = 6.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in smog chamber (Nolting et al. 1988)

k_{OH}* = 5.61 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1991, Altshuller 1991)

k_{OH} = 5.58 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 1.05 × 10^{-16} cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

k_{OH} = 5.61 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, k_{NO3} = 10.5 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

k_{NO3} = 1.05 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (Atkinson 1991)

k_{NO3}(exptl) = 1.06 × 10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) = 1.11 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 5.45 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 11 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

k_{OH}* = 5.19 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction $t_{1/2}$ = 2.4–24 h in air, based on reaction rate constant of 3.8 × 10^9 L mol^{-1} s^{-1} for the reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric lifetime ~ 25 h, based on a rate constant of 5.61 × 10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with OH radicals in summer daylight (Altshuller 1991).

TABLE 2.1.1.1.16.1
Reported aqueous solubilities of *n*-hexane at various temperatures

1.

Nelson & De Ligny 1968		Polak & Lu 1973		Price 1976		Jönsson et al. 1982	
shake flask-GC		shake flask-GC		shake flask-GC		vapor saturation-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
4.0	16.4	0	16.5	25.0	9.47	15	10.72
14.0	15.2	25	12.4	40.1	10.1	20	10.32
25.0	18.3			55.7	13.2	25	10.09
35.0	12.9			69.7	15.4	30	10.02
45.0	22.2			69.7	15.2	35	10.10
55.0	21.2			99.1	22.4		
				114.4	29.2		
				121.3	37.6		
				137.3	56.9		
				151.8	106.0		

(*Continued*)

TABLE 2.1.1.1.16.1 (*Continued*)

2.

Tsonopoulos & Wilson 1983		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		IUPAC recommended		calc-recommended LLE	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
37.78	11.4	0	17	0	15.8
93.33	27.4	20	12	4	14.36
94.4	25.6	24	11	13	12.45
100	29.7	30	9.9	15	12.45
148.09	130	40	11	20	12.0
150	162	50	12	25	11.5
200	885	60	13.6	30	11.5
		70	15.7	35	11.5
		80	18.5	40.1	11.5
		100	27	55.7	12.93
		120	45	69.7	15.32
		140	80	99.1	26.33
				113.8	37.34
				121.3	44.52
				137.2	67.02
				151.8	105.3

FIGURE 2.1.1.1.16.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *n*-hexane.

TABLE 2.1.1.1.16.2
Reported vapor pressures of *n*-hexane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad\qquad \ln P = A - B/(T/K) \quad (1a)$$
$$\log P = A - B/(C + t/°C) \quad (2) \qquad \ln P = A - B/(C + t/°C) \quad (2a)$$
$$\log P = A - B/(C + T/K) \quad (3) \qquad \ln P = A - B/\{(T/K) - C\} \quad (3a)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$
$$\ln [(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\} \quad (5) \text{ - Cox eq.}$$

1.

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-manometer		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30	24811	13.033	11698	−53.9	133.3	−25.19	1333
40	36757	16.576	13819	−34.5	666.6	−14.36	2666
50	53409	20.618	16620	−25.0	1333	−7.50	4000
60	75727	24.717	19920	−14.1	2666	−2.36	5333
		28.528	23451	−2.30	5333	1.79	6666
bp/°C	68.8	33.631	28956	5.40	7999	5.31	7999
		38.311	34896	15.8	13332	11.08	10666
		43.967	43322	31.6	26664	15.762	13332
		49.803	53655	49.8	53329	24.764	19998
		56.030	66757	68.7	101325	31.572	26664
		62.785	83719			37.114	33331
		67.554	97605	mp/°C	−95.3	41.824	39997
		68.067	99201			49.612	53329
		68.540	100694			55.973	66661
		69.081	102394			61.394	79993
		69.541	103913			66.145	93326
						67.030	95992
		bp/°C	68.740			67.896	98659
						68.744	101325
		eq. 2	P/mmHg				
		A	6.87776			eq. 2	P/mmHg
		B	1171.530			A	6.87024
		C	224.366			B	118.72
		temp range: 13–69.5°C				C	224.210
						bp/°C	68.744
						$\Delta H_v/(kJ\ mol^{-1})$ =	
						at 25°C	31.55
						at bp	28.85

(Continued)

TABLE 2.1.1.1.16.2 (*Continued*)

2.

Carruth & Kobayashi 1973		Letcher & Marsicano 1974		Gracia et al. 1992		Ruzicka & Majer 1994	
gas saturation		static method-manometer		Hg manometer		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–95.44	1.360	27.11	22091	9.95	10081	162.54	0.1
–95.13	1.373	29.31	24151	14.98	12818	176.70	1.0
–91.70	2.266	33.81	29197	19.97	16136	193.88	10
–88.93	3.213	36.44	32437	24.96	20136	215.51	100
–83.99	5.973	39.88	37117	29.96	24949	243.81	1000
–75.94	13.60	42.45	40996	34.95	30577	282.95	10000
–61.25	64.13	45.15	45289	39.93	37185	341.863	101325
–53.29	128	48.11	50476	44.96	45000	298.15	20180
–34.84	656			49.97	54028		
–24.91	1264	Antoine eq.				data calc. from Cox eq.	
–14.39	2560	eq. 3	P/mmHg			eq. 5	P/kPa
–0.51	3120	A	6.6298	Antoine eq.		A_0	2.73425
		B	1050.38	eq. 3a	P/kPa	A_1	2.02283×10^{-3}
mp/°C	–95.36	C	210.477	A	13.74029	A_2	2.287564×10^{-6}
				B	2654.670	with reference state at	
eq. 1a	P/mmHg	$\Delta H_V/(kJ\ mol^{-1}) = 30.84$		C	50.869	P_o/kPa	101.325
A	19.5553					T_o/K	341.863
B	4292.8						

FIGURE 2.1.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexane.

TABLE 2.1.1.1.16.3

Reported Henry's law constants and octanol-air partition coefficients of *n*-hexane 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)	$\log [H/(atm \cdot m^3/mol)] = A - B/(T/K)$ (4a)
$\ln [H/(Pa\ m^3/mol)] = A - B/(T/K)$	(4)	
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)	

Henry's law constant							log K_{OA}	
Jönsson et al. 1982		Ashworth et al. 1988		Kolb et al. 1992			Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		equilibrium headspace-GC			GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)		t/°C	log K_{OA}
14.52	103536	10	24115	40	18600		20.29	2.548
14.52	103090	15	41847	60	64410		30.3	2.386
15.0	103262	20	89470	70	237750		40.4	2.216
20.05	135426	25	77818				50.28	2.090
20.05	136182	30	158067	eq. 2	1/K_{AW}			
20.0	135403			A	−28.60			
25	174565	eq. 4	H/(atm m³/mol)	B	−8375			
25	172140	A	25.25					
25	172140	B	7530					
30.2	215560							
30.2	211937							
30.0	215418							
34.9	264034							
34.9	256113							
35.0	261424							
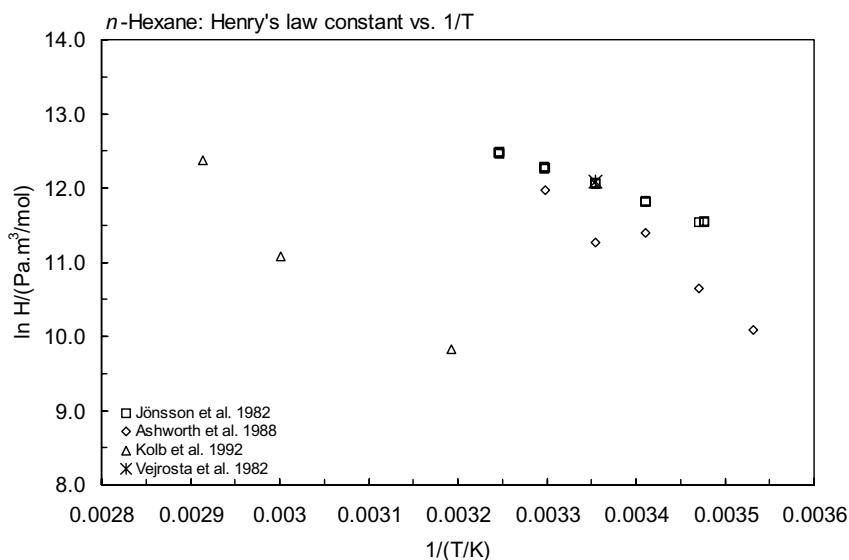
FIGURE 2.1.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-hexane.
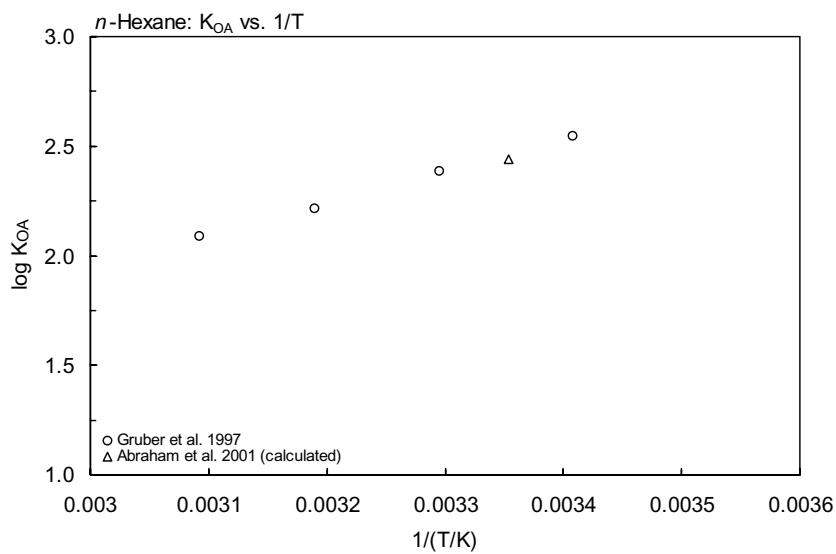
FIGURE 2.1.1.1.16.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-hexane.

2.1.1.1.17   2-Methylhexane (Isoheptane)
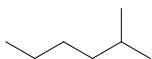
Common Name: 2-Methylhexane
Synonym: isoheptane, ethylisobutylmethane
Chemical Name: 2-methylhexane
CAS Registry No: 591-76-4
Molecular Formula: C_7H_{16}; $CH_3CH(CH_3)CH_2(CH_2)_2CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –118.2   (Lide 2003)
Boiling Point (°C):
    90.04   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6786, 0.6744   (20°C, 25°C, Dreisbach 1959)
    0.6786, 0.6548   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    147.66, 148.58   (20°C, 25°C, calculated-density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    34.807, 30.669   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.184   (Dreisbach 1959; Riddick et al. 1986)
    9.18   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    59.29, 57.8   (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    2.54   (shake flask-GC, Price 1976)
    3.51   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    8380   (calculated-Antoine eq. regression, temp range –40.4 to 90°C, Stull 1947)
    9000   (25.518°C, ebulliometry, measured range 18.5–90.9°C, Forziati et al. 1949)
    log (P/mmHg) = 6.87319 – 1236.026/(219.545 + t/°C); temp range (Antoine eq., ebulliometry-manometer
        measurements, Forziati et al. 1949)
    8780   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.87318 – 1236.026/(219.545 + t/°C); temp range 10–110°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    8780   (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 5.87318 – 1236.026/(219.545 + t/°C); temp range –9.10 to 114.78°C (Antoine eq., Zwolinski
        & Wilhoit 1971)
    8370   (interpolated-Antoine eq., Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 8538.7/(T/K)] + 8.055523; temp range –40.4 to 90°C (Antoine eq., Weast 1972–73)
    87778, 8785 (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.0031 – 1238.614/(219.867 + t/°C); temp range 18.5–90.9°C (Antoine eq. from reported exptl.
        data of Forziati et al. 1949, Boublik et al. 1984)
    log (P/kPa) = 6.06712 – 1270.535/(222.971 + t/°C); temp range 0–45°C (Antoine eq. from reported exptl. data,
        Boublik et al. 1984)
    8790   (interpolated-Antoine eq., temp range –9 to 115°C, Dean 1985, 1992)
    log (P/mmHg) = 6.87318 – 1236.026/(219.55 + t/°C); temp range –9 to 115°C (Antoine eq., Dean 1985, 1992)

8800   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.99612 – 1235.10/(219.469 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

8790   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.00513 – 1240.11/(–53.123 + T/K); temp range 296–365 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 54.1075 – 3.785 × 10^3/(T/K) – 17.547·log (T/K) + 8.2594 × 10^{-3}·(T/K) – 3.4967 × 10^{-14}·(T/K)^2; temp range 155–530 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.):

346000   (calculated-P/C, Mackay & Shiu 1981, Eastcott et al. 1988)

346500   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

51878*   (26.9°C, EPICS-GC, measured range 26.9–45°C, Hansen et al. 1993)

ln [H/(kPa·m^3/mol)] = 3608/(T/K) – 8.0; temp range 26.9–45°C (EPICS-GC, Hansen et al. 1993)

63856   (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

log K$_{AW}$ = –4.274 + 1669/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

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

k$_{OH}$ = 6.80 × 10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson 1990, 1991)

k$_{OH}$ = 6.80 × 10^{-12} cm^3 molecule^{-1} s^{-1} with atmospheric lifetime of 25 h in summer daylight (Altshuller 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 6.80 × 10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radicals and an estimated lifetime of 25 h in summer daylight (Altshuller 1990).

TABLE 2.1.1.1.17.1
Reported Henry's law constants of 2-methylhexane at various temperatures

Hansen et al. 1993	
EPICS-GC	
t/°C	H/(kPa m^3/mol)
26.9	51.878
35.0	31.512
45.0	25.939
ln [H/(Pa m3/mol)] = A – B/(T/K)	
eq. 4	H/(kPa m^3/mol)
A	–8 ± 3.53
B	–3608 ± 1088

2.1.1.1.18   3-Methylhexane
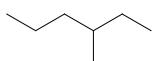
Common Name: 3-Methylhexane
Synonym: ethylmethylpropylmethane
Chemical Name: 3-methylhexane
CAS Registry No: 589-34-4
Molecular Formula: C_7H_{16}; $CH_3CH_2CH(CH_3)(CH_2)_2CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –119.4   (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
    92   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6860   (Weast 1984)
    0.6871, 0.6830   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    145.83, 146.71   (calculated-density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    35.087, 30.79 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    4.95   (shake flask-GC, Polak & Lu 1973)
    2.64   (shake flask-GC, Price 1976)
    3.80   (suggested IUPAC tentative value, Shaw 1989)
    6.12, 4.29   (0. 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    7782   (Antoine eq. regression, temp range –39 to 91.9°C Stull 1947)
    7702   (23.662°C, ebulliometry, measured range 19.915–92.737°C, Forziati et al. 1949)
    log (P/mmHg) = 6.86754 – 1240.196/(219.223 + t/°C); temp range 19.9–92.7°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
    8210   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.86764 – 1240.196/(219.223 + t/°C); temp range 10–130°C (Antoine eq. for liquid state, Dreisbach 1959)
    8213   (interpolated-Antoine eq., temp range –7.90 to 116.73°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.86764 – 1240.196/(219.223 + t/°C); temp range –7.90 to 116.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
    7772   (interpolated-Antoine eq., temp range –39.0 to 91.9°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 8596.3/(T/K)] + 8.065472; temp range –39.0 to 91.9°C (Antoine eq., Weast 1972–73)
    8212   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.99489 – 1241.528/(219.375 + t/°C); temp range 20–92.74°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
    8210   (interpolated-Antoine eq., temp range –8 to 117°C Dean 1985, 1992)
    log (P/mmHg) = 6.86764 – 1240.196/(219.22 + t/°C); temp range –8 to 117°C (Antoine eq., Dean 1985, 1992)
    8300   (lit. average, Riddick et al. 1986)
    log (P/kPa) = 5.98993 – 1238.88/(219.10 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    8215   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.9926 – 1239.57/(–53.979 + T/K); temp range 289–366 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 35.2535 – 2.931 × 10^3/(T/K) – 9.667·log (T/K) – 5.2026 × 10^{-11}·(T/K) + 3.2107 × 10^{-6}·(T/K)^2; temp range 154–535 K (vapor pressure eq., Yaws 1994)

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

172000   (recommended, Mackay & Shiu 1981)
312170   (calculated-P/C, Eastcott et al. 1988)
311620   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: 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} = 7.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990,1991)
k_{OH} = 7.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime of 20 h during summer daylight (Altshuller 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
photooxidation reaction rate constant of 7.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radical and an estimated lifetime of 20 h during summer daylight (Altshuller 1991).

2.1.1.1.19   2,2,5-Trimethylhexane
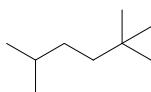

Common Name: 2,2,5-Trimethylhexane
Synonym:
Chemical Name: 2,2,5-trimethylhexane
CAS Registry No: 3522-94-9
Molecular Formula: C_9H_{20}, $(CH_3)_3CCH_2CH_2CH(CH_3)_2$
Molecular Weight: 128.255
Melting Point (°C):
    –105.7   (Lide 2003)
Boiling Point (°C):
    124.09   (Lide 2003)
Density (g/cm³ at 25°C):
    0.7072   (Weast 1984)
    0.7072, 0.7032   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    181.3, 182.4   (20°C, 25°C, calculated-density)
    207.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    40.175, 33.76 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.192   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    1.15   (shake flask-GC, McAuliffe 1966)
    0.79; 0.54, 0.54   (0; 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
    0.80, 0.80   (0, 25°C, IUPAC recommended best value, Shaw1989b)
    0.613   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    log (P/mmHg) = 6.83532 – 1324.049/(210.737 + t/°C); temp range 46.1–125.0°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
    2212   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.83531 – 1324.059/(210.737 + t/°C); temp range 35–145°C (Antoine eq. for liquid state, Dreisbach 1959)
    2210   (interpolated-Antoine eq., temp range 16.17–151.1°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.83531 – 1324.049/(210.737C + t/°C); temp range 16.17–151.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
    2216   (static method-inclined piston manometer, measured range –35 to 30°C, Osborn & Douslin 1964)
    2207   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.96385 – 1326.27/(212.991 + t/°C); temp range 46.14–126.05°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
    2207   (extrapolated-Antoine eq., temp range 46 to 125°C Dean 1985, 1992)
    log (P/mmHg) = 6.83775 – 1325.54/(210.91 + t/°C); temp range 46–125°C (Antoine eq., Dean 1985, 1992)
    2216   (lit. average, Riddick et al. 1986)
    log (P/kPa) = 5.96021 – 1324.049/(210.737 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    2218   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.99253 – 1243.85/(–60.158 + T/K); temp range 288–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.25179 - 1471.621/(-48.901 + T/K)$; temp range 238–293 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/mmHg) = 7.8816 - 2.6422 \times 10^3/(T/K) + 23.902 \cdot \log (T/K) - 1.5376 \times 10^{-2} \cdot (T/K) + 7.7931 \times 10^{-6} \cdot (T/K)^2$; temp range 167–568 K (vapor pressure eq., Yaws 1994)

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

350000   (recommended, Mackay & Shiu 1981)

523760   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

4.63   (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.46   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants and Half-Lives:

Half-Lives in the Environment:

2.1.1.1.20   n-Heptane
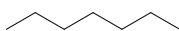
Common Name: *n*-Heptane
Synonym: heptane
Chemical Name: *n*-heptane
CAS Registry No: 142-82-5
Molecular Formula: C_7H_{16}, $CH_3(CH_2)_5CH_3$
Molecular Weight: 100.202
Melting Point (°C):
    –90.55   (Lide 2003)
Boiling Point (°C):
    98.4   (Dreisbach 1959; Weast 1972–73; Lide 2003)
Density (g/cm^3 at 20°C):
    0.6837   (Weast 1972–73)
    0.6837, 0.6795   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    146.6, 147.5 (20°C, 25°C, calculated-density)
    162.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    36.55, 31.7 (25°C, bp, Riddick et al. 1986)
    36.57   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    14.037   (Riddick et al. 1986)
    14.04   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    76.9, 81.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    50.0   (15.5°C, shake flask-cloud point, Fühner 1924)
    150   (radiotracer method, Black et al. 1948)
    15.0   (16°C, shake flask-cloud point, Durand 1948)
    2.93   (shake flask-GC, McAuliffe 1963,1966)
    11.0*   (22°C, cloud point, measured range 295–355 K at 17–55 MPa, Connolly 1966)
    2.66*   (shake flask-GC, measured range 4.3–45°C, Nelson & De Ligny 1968)
    4.39; 3.37* (0, 25°C, shake flask-GC, Polak & Lu 1973)
    2.57   (shake flask-GC, Krasnoshchekova & Gubertritis 1975)
    2.24*   (shake flask-GC, measured range 25–150.4°C, Price 1976)
    3.70   (shake flask-GC, Bittrich et al. 1979)
    2.90   (partition coefficient-GC, Rudakov & Lutsyk 1979)
    3.58   (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)
    4.62   (calculated-activity coeff. γ and K_{OW}, Tewari et al. 1982b)
    2.51*   (vapor saturation-GC, measured range 15–40°C, Jönsson et al. 1982)
    2.95   (shake flask-GC, Coates et al. 1985)
    3.57   (lit. average, Riddick et al. 1986)
    2.90   (shake flask-purge and trap-GC, Coutant & Keigley 1988)
    2.40*   (recommended best value, IUPAC Solubility Data Series, temp range 0–140°C, Shaw 1989)
    $\ln x = -396.93979 + 17232.298/(T/K) + 56.95927 \cdot \ln (T/K)$, temp range 290–400 K (eq. derived from literature
        calorimetric and solubility data, Tsonopoulos 1999)
    2.95*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–423.6 K, Mączyński et al. 2004)

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

5520*   (22.7°C, static-manometer, measured range 22.7–98.4°C, Smyth & Engel 1929)

6370*   (25.9°C, ebulliometry, measured range 25.9–99.3°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.90342 - 1268.636/(216.951 + t/°C)$; temp range 25.9–99.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

5795*   (calculated-Antoine eq. regression, temp range –34 to 98.4°C Stull 1947)

6425*   (26.039°C, ebulliometry, measured range 26–99.3°C Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.90027 - 1296.871/(216.757 + t/°C)$; temp range 26.0–99.3°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

6110   (calculated from determined data, Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.90240 - 1268.115/(216.90 + t/°C)$; temp range 15–155°C (Antoine eq. for liquid state, Dreisbach 1959)

6105   (Harris & Dunlop 1970)

6113*   (interpolated-Antoine eq., temp range –2.10 to 123.41°C, Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.90240 - 1268.115/(216.900 + t/°C)$; temp range –2.10 to 123.41°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 8409.6/(T/K)] + 7.786586$; temp range –34.0 to 247.5°C (Antoine eq., Weast 1972–73)

5080*   (22.46°C, gas saturation, measured range –87.85 to 22.46°C, Carruth & Kobayashi 1973)

6037, 6057 (static method-differential pressure gauge, Bissell & Williamson 1975)

7826, 18929, 40469, 57059(30, 50, 70, 80°C, vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)

6090   (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.02701 - 1167.592/(216.796 + t/°C)$; temp range 25.92–99.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 4.38001 - 668.768/(159.522 + t/°C)$; temp range –87.85 to 22.4°C (Antoine eq. from reported exptl. data of Carruth & Kobayashi 1973, Boublik et al. 1984)

6110, 5958, 6090   (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)

6090   (interpolated-Antoine eq., temp range –2 to 124°C Dean 1985. 1992)

$\log (P/\text{mmHg}) = 6.98677 - 1264.90/(216.54 + t/°C)$; temp range –2 to124°C (Antoine eq., Dean 1985, 1992)

6090   (literature average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.02167 - 1264.90/(216.544 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

6110   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.02633 - 1268.583/(-56.054 + T/K)$; temp range 297–375 K (Antoine eq., Stephenson & Malanowski 1987)

6102*   (recommended, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{2.86470 - 2.113204 \times 10^{-3} \cdot (T/K) + 2.250991 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 371.552$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 65.0257 - 3.8188 \times 10^3/(T/K) -21.684 \cdot \log (T/K) + 1.0387 \times 10^{-2} \cdot (T/K) + 1.0206 \times 10^{-14} \cdot (T/K)^2$; temp range 183–540 K (vapor pressure eq., Yaws 1994)

12309   (40°C, average value, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)

7811, 18869 (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

62503*   (355.899 K, ebulliometry, measured range 355.899–503.406 K, Weber 2000)

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.):

206200   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

226000, 73120   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

230000   (recommended, Mackay & Shiu 1981)

250420*   (25.04°C, equilibrium cell-concentration ratio-GC, measured range 15.3–35.05°C Jönsson et al. 1982)

136120, 184640, 243020, 315050, 394150(15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)

ln $1/K_{AW}$ = 23748.4/(T/K) + 64.927·ln (T/K) – 454.172; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

273400   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

91294*   (26°C, EPICS-GC, measured range 26–45°C, Hansen et al. 1993)

ln [H/(kPa·m^3/mol)] = –3730/(T/K) + 17.0; temp range 26–45°C (EPICS-GC, Hansen et al. 1993)

220825   (EPICS-GC, Ryu & Park 1999)

68000   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 6.532 – 1491/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

3.50   (calculated-π constant, Hansch et al. 1968, Hansch & Leo 1979)

4.76   (calculated-activity coeff. γ, Wasik et al. 1981,1982)

4.66   (generator column-GC, Tewari et al. 1982a,b)

3.44   (HPLC-k′ correlation, Coates et al. 1985)

4.48   (Berti et al. 1986)

4.66, 4.72   (generator column-GC, calculated-activity coeff. γ, Schantz & Martire 1987)

4.50 ± 0.25   (recommended, Sangster 1989)

4.66   (recommended, Sangster 1993)

4.99   (calculated-activity coefficients, Tse & Sandler 1994)

4.66   (recommended, Hansch et al. 1995)

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

3.05*   (20.29°C, from GC-determined γ° in octanol, measured range 20.29–50.28°C Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = (7.30 ± 0.17) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 299 ± 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

k_{NO3} = 1.36 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1988,1990)

k_{OH} = 7.52 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in smog chamber (Nolting et al. 1988)

k_{OH}* = 7.15 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1991)

k_{OH} = 7.15 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, k_{NO3} = 1.36 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

k_{OH} = 7.19 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 1.36 × 10^{-16} cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

k_{OH} = 7.15 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K, with a calculated atmospheric lifetime of 19 h during summer daylight hours (Altshuller 1991)

k_{NO3} = (1.34 – 1.37) × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1991)

k_{NO3}(exptl) = (1.36, 1.38) × 10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO3}(recommended) = 1.37 × 10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) = 1.45 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 7.02 × 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 15 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 7.15×10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radicals with an estimated lifetime of 19 h in summer daylight (Altshuller 1991).

TABLE 2.1.1.1.20.1
Reported aqueous solubilities of *n*-heptane at various temperatures

1.

Connolly 1966		Nelson & De Ligny 1968		Polak & Lu 1973	
shake flask-cloud point		shake flask-GC		shake flask-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
22	1.1	4.3	1.95	0	4.39
57	3.3	13.5	2.02	25	3.37
77	3.7	25.0	2.66		
82	10.3	35.0	2.27		

2.

Price 1976		Jonsson et al. 1982		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		vapor saturation-GC		IUPAC "tentative" best values		calc-recommended LLE data	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
25.0	2.24	15	2.67	0	3.0	0	4.18
40.1	2.63	20	2.57	10	2.0	15	3.23
55.7	3.11	25	2.51	20	2.4	20	3.06
99.1	5.60	30	2.49	25	2.4	25	2.95
118.0	11.4	35	2.52	30	2.40	30	2.90
136.6	27.3			40	2.5	35	2.90
150.4	43.7			50	2.9	40.1	2.95
				60	3.3	45	3.01
				90	3.9	55.7	3.34
				100	5.8	99.1	7.79
				120	13	118	12.8
				140	31	136.6	22.8
						150.4	36.7
				ΔH_{sol}/(kJ mol^{-1}) = –2.43			
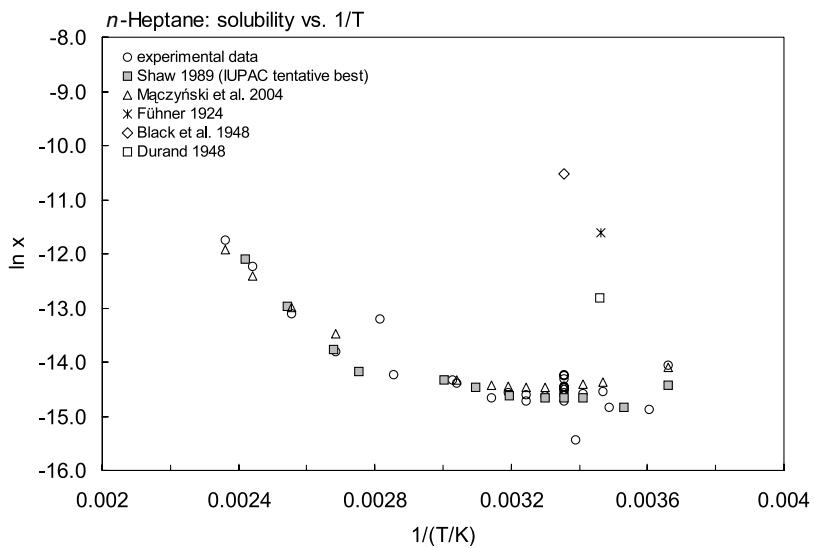
FIGURE 2.1.1.1.20.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *n*-heptane.

TABLE 2.1.1.1.20.2
Reported vapor pressures of *n*-heptane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln [(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\}$			(5) - Cox eq.

1.

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
static method-manometer		ebulliometry		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
22.7	5520	25.925	6370	–34.0	133.3	26.030	6425
30.0	7759	29.699	7665	–12.7	666.6	29.813	7717
30.3	7839	33.024	8977	–2.1	1333	33.108	9013
38.4	11466	36.017	10311	9.5	2666	36.105	10352
50.0	18812	38.822	11700	22.3	5333	38.901	11740
51.2	19998	42.599	13821	30.6	7999	42.680	13866
61.2	29331	46.929	16604	41.8	13332	46.987	16659
69.5	39703	51.320	19920	58.7	26664	51.373	19966
70.0	40183	55.394	23443	78.0	53329	55.442	23499
79.5	55955	60.862	28950	98.4	101325	60.902	29003
98.4	101325	65.882	34897			65.916	34948
		71.930	43326	mp/°C	–90.6	71.966	43386
mp/°C	–90.5	78.160	53647			78.202	53270
bp/°C	98.4	84.823	66749			84.856	66815
		92.053	83706			92.678	83769
		97.154	97590			97.180	97663
		97.702	99186			97.728	99257
		98.207	100689			98.237	100758

(*Continued*)

TABLE 2.1.1.1.20.2 *(Continued)*

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
static method-manometer		ebulliometry		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		98.773	102393			98.813	102476
		99.285	103907			99.322	104018
		bp/°C	98.426			bp/°C	98.427
		eq. 2	P/mmHg				
		A	6.90342			eq. 2	P/mmHg
		B	1268.636			A	6.90027
		C	216.951			B	1266.871
		temp range: 25.9–99.3°C				C	216.757
						temp range: 26.0–99.3°C	

2.

Zwolinski & Wilhoit 1971		Carruth & Kobayashi 1973		Ruzicka & Majer 1994		Weber 2000	
selected values		gas saturation		recommended		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–2.22	1333	–87.85	0.288	–40	76.3	355.899	62503
9.43	2666	–80.41	0.867	–20	393	359.210	69482
16.78	4000	–68.21	4.240	0	1520	363.492	79475
22.29	5333	–55.70	16.40	20	4730	367.925	89500
26.75	6666	–42.11	57.46	25	6102	370.925	99446
30.519	7999	–27.95	196	40	12300	374.219	109546
36.706	10666	–14.0	595	60	28100	377.268	119434
41.723	13332	1.01	1667	80	57100	380.130	129452
51.366	19998	11.92	2986	100	106000	382.836	139321
58.656	26664	22.46	5080			386.617	154371
64.591	33331			OR		390.085	169321
69.632	39997	mp/°C	–90.60	T/K	P/Pa	394.397	189252
77.966	53329			179.40	0.1	335.188	30303
84.772	66661	eq. 1a	P/mmHg	194.52	1.0	339.317	35308
90.571	79993	A	20.1590	212.98	10	342.996	40310
95.650	93326	B	4852.65	236.18	100	349.358	50269
96.597	95992			266.53	1000	352.183	55286
97.523	98659			308.48	10000	354.804	60285
98.429	101325			371.55	101325	357.252	65269
				298.15	6102	359.559	70277
eq. 2	P/mmHg					363.894	60452
A	6.89385			data calc. from Cox eq.		367.733	90423
B	1264.37			eq. 5	P/kPa	371.255	100423
C	216.636			A_0	2.86470	374.510	110415
bp/°C	98.429			A_1	2.113204×10^{-3}	377.544	120394
$\Delta H_V/(kJ\ mol^{-1})$ =				A_2	2.250991×10^{-6}	380.390	130382
at 25°C	36.55			with reference state at		383.069	140381
at bp	31.70			P_o/kPa	101.325	386.826	155364
				T_o/K	371.552	390.313	170377
						394.609	190385
						to	
						503.406	1597746
						see ref. for complete set of data	
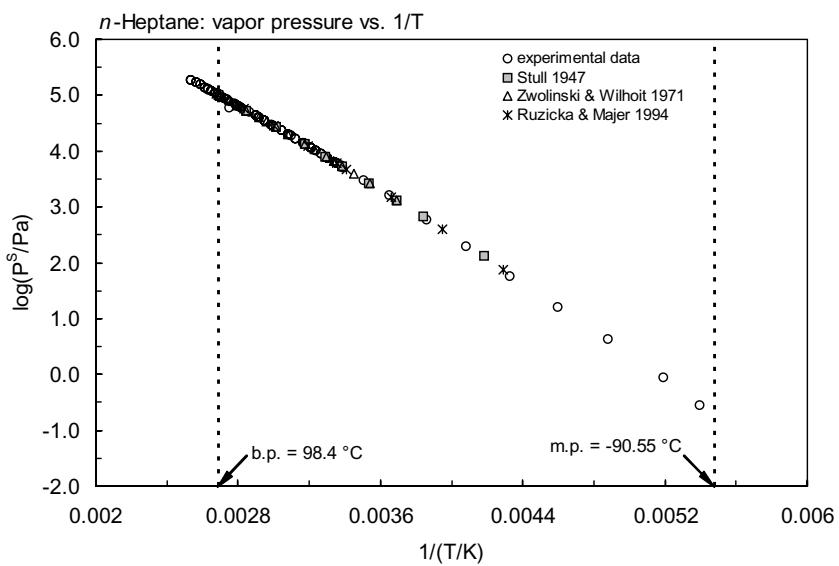
FIGURE 2.1.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-heptane.

TABLE 2.1.1.1.20.3
Reported Henry's law constants and octanol-air water partition coefficients of *n*-heptane 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)	

Henry's law constant				log K_OA	
Jönsson et al. 1982		Hansen et al. 1993		Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	log K_OA
15.0	136118*	26.0	91294	20.29	3.047
15.3	140244	35.8	121083	30.3	2.839
15.3	136260	45.0	193024	40.4	2.654
20.0	184640*			50.28	2.510
20.05	190443	eq. 4	H/(kPa m³/mol)		
20.05	187513	A	17 ± 2.22		
25.0	243021*	B	3730 ± 686		
25.05	193690				
25.05	190710				
25.04	250419				
29.8	302857				
29.8	316821				
30.0	315049*				
35.05	389419				
34.83	405792				
34.83	379903				
35.0	394148*				
* interpolated data					
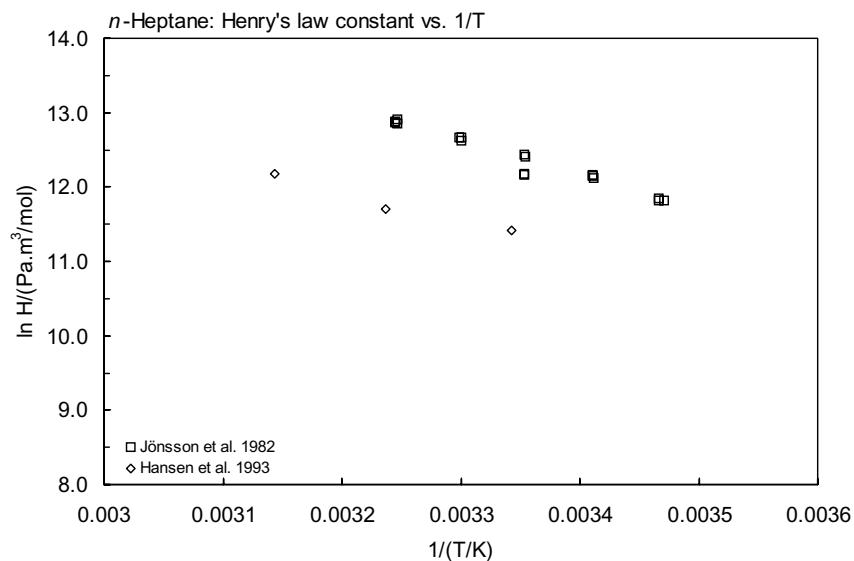
FIGURE 2.1.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-heptane.
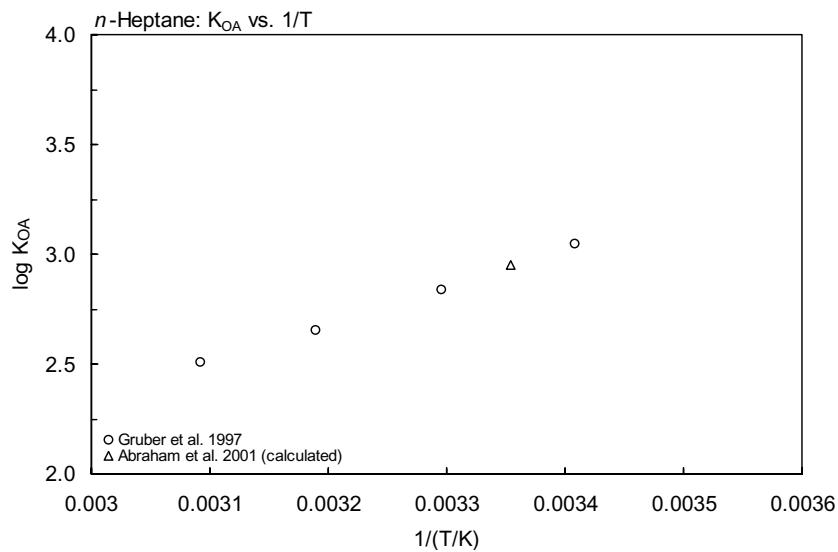
FIGURE 2.1.1.1.20.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-heptane.

2.1.1.1.21   2-Methylheptane
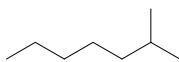
Common Name: 2-Methylheptane
Synonym:
Chemical Name: 2-methylheptane
CAS Registry No: 592-27-8
Molecular Formula: C_8H_{18}; $CH_3CH(CH_3)(CH_2)_4CH_3$
Molecular Weight: 114.229
Melting Point (°C):
     –109.02   (Lide 2003)
Boiling Point (°C):
     117.66   (Lide 2003)
Density (g/cm³ at 20°C):
     0.698   (Lide 2003)
Molar Volume (cm³/mol):
     163.7   (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
     185.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     39.68, 33.60 (25°C, normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     11.92   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     72.62, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
     0.95, 4.55   (quoted, calculated-molar volume V_M, Wang et al. 1992)
     2.84; 5.94   (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
     0.95; 1.61, 1.61   (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
     log (P/mmHg) = 6.91737 – 1337.468/(213.693 + t/°C); temp range 41.7–118.5°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
     2620   (calculated-Antoine eq. regression, temp range –21 to 117.6°C Stull 1947)
     6386   (23.4°C, Nicolini & Laffitte 1949)
     2748   (extrapolated-Antoine eq., Dreisbach 1959)
     log (P/mmHg) = 6.91735 – 1337.468/(213.693 + t/°C); temp range 35–150°C (Antoine eq. for liquid state, Dreisbach 1959)
     2748   (interpolated-Antoine eq., temp range 12.3–143.8°C, Zwolinski & Wilhoit 1971)
     log (P/mmHg) = 6.91735 – 1337.468/(213.693 + t/°C); temp range 12.3–143.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
     2620   (interpolated-Antoine eq., temp range –21–117.6°C, Weast 1972–73)
     log (P/mmHg) = [–0.2185 × 9362.0/(T/K)] + 8.154424; temp range –21–117.6°C (Antoine eq., Weast 1972–73)
     2732, 6850 (calculated-Antoine eq., Boublik et al. 1973, 1984)
     log (P/mmHg) = 6.88814 – 1319.539/(211.625 + t/°C); temp range 41–118.5°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)
     log (P/mmHg) = 6.85999 – 1313.125/(230.02 + t/°C); temp range 23.4–75°C (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1973)
     1161   (10°C, static method-inclined piston manometer, measured range –40 to 10°C, Osborn & Douslin 1974)

2750   (extrapolated-Antoine eq., temp range 42–119°C, Dean 1985, 1992)
log (P/mmHg) = 6.91735 – 1337.47/(213.69 + t/°C); temp range 42–119°C (Antoine eq., Dean 1985, 1992)
2750   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P$_L$/kPa) = 6.05858 – 1346.996/(–30.648 + T/K); temp range 285–392 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P$_L$/kPa) = 6.81199 – 1703.6/(–30.648 + T/K); temp range 233–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 37.693 – 3.2611 × 10^3/(T/K) – 10.391·log (T/K) – 1.0524 × 10^{-12}·(T/K) + 3.056 × 10^{-6}·(T/K)^2; temp range 164–560 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
369880   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K$_{OW}$:
3.91   (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
4.04   (calculated-V$_M$, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

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

Environmental Fate Rate Constants, k, and Half-Lives, t$_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: 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$_{OH}$(calc) = 8.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} (SAR structure reactivity relationship, Atkinson 1987)
        k$_{OH}$ = 8.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} with a calculated atmospheric lifetime τ = 17 h during summer daylight hours (Altshuller 1991).
    Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
    Air: photooxidation reaction rate constant of 8.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radical and an estimated lifetime of 17 h during summer daylight (Altshuller 1991).

2.1.1.1.22   3-Methylheptane
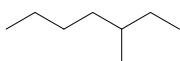
Common Name: 3-Methylheptane
Synonym:
Chemical Name: 3-methylheptane
CAS Registry No: 589-81-1
Molecular Formula: C_8H_{18}; $CH_3CH_2CH(CH_3)(CH_2)_3CH_3$
Molecular Weight: 114.229
Melting Point (°C):
    –120.48   (Lide 2003)
Boiling Point (°C):
    118.9   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7075   (Weast 1984)
    0.7058, 0.7018   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    161.4   (20°C, calculated-density, Stephenson & Malanowski 1987)
    185.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    39.83, 34.08   (25°C, normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    11.38   (Dreisbach 1959)
    11.7   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    76.6, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.792   (shake flask-GC, Price 1976; quoted, Mackay & Shiu 1981; Shaw 1989; Myrdal et al. 1992)
    0.850   (estimated-nomograph, Brookman et al. 1985)
    1.015   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    log (P/mmHg) = 6.89945 – 1331.530/(212.414 + t/°C); temp range 42.7–119.8°C (Antoine eq. from exptl. data, ebulliometry, manometer, Willingham et al. 1945)
    2610   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.89944 – 1331.530/(212.414 + t/°C); temp range 30–150°C (Antoine eq. for liquid state, Dreisbach 1959)
    2600   (interpolated-Antoine eq., temp range 13.3–145.2°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.89944 – 1331.530/(212.414 + t/°C); temp range 13.3–145.2°C (Antoine eq., Zwolinski & Wilhoit 1971)
    2466   (interpolated-Antoine eq., temp range –19.8 to 118.9°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 9432.0/(T/K)] + 8.179407; temp range –19.8 to 118.9°C (Antoine eq., Weast 1972–73)
    1486   (15°C, static method-inclined piston manometer, measured range –35 to 15°C, Osborn & Douslin 1974)
    2600, 3232 (quoted, calculated-bp, Mackay et al. 1982)
    2600   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.01647 – 1326.329/(211.776 + t/°C); temp range 42.67–119.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
    2605   (extrapolated, Antoine eq., temp range 43–120°C Dean 1985, 1992)
    log (P/mmHg) = 6.89944 – 1331.53/(212.41 + t/°C); temp range 43–120°C (Antoine eq., Dean 1985, 1992)

2630   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.02047 - 1329.42/(-60.945 + T/K)$; temp range 286–393 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.50909 - 1567.45/(-40.786 + T/K)$; temp range 238–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/mmHg) = 52.8828 - 3.6231 \times 10^3/(T/K) - 16.804 \cdot \log(T/K) + 7.1828 \times 10^{-3} \cdot (T/K) + 7.4077 \times 10^{-14} \cdot (T/K)^2$; temp range 153–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol):

376000   (calculated-P/C, Mackay & Shiu 1981)

375900   (selected, Mills et al. 1982)

375800   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

Oxidation: 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}(calc) = 8.90×10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987)

$k_{OH} = 8.90 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with a calculated atmospheric lifetime $\tau = 16$ h during summer daylight hours (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 8.90×10^{-12} cm³ molecule⁻¹ s⁻¹ with hydroxyl radical with an estimated lifetime of 16 h during summer daylight (Altshuller 1991).

2.1.1.1.23   n-*Octane*

Common Name: *n*-Octane
Synonym: octane
Chemical Name: *n*-octane
CAS Registry No: 111-65-9
Molecular Formula: C_8H_{18}; $CH_3(CH_2)_6CH_3$
Molecular Weight: 114.229
Melting Point (°C):
    −56.82   (Lide 2003)
Boiling Point (°C):
    125.67   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7027, 0.6886   (20°C, 25°C, Riddick et al. 1986)
    0.70256   (20°C, digital precision densimeter, Dejoz et al. 1996)
Molar Volume (cm³/mol):
    162.6, 165.8 (20°C, 25°C, calculated-density)
    185.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.49, 34.431   (25°C, bp, Riddick et al. 1986)
    41.56   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    20.74   (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    95.86, 91.1 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    14.0   (cloud point, Fühner 1924, quoted, Deno & Berkheimer 1960)
    0.66   (shake flask-GC, McAuliffe 1963, 1966)
    0.493   (radiotracer method, Baker 1967)
    0.880*   (shake flask-GC, measured range 5–25°C, Nelson & De Ligny 1968)
    0.700   (shake flask-GC, Krznoshchekova & Gubergrits 1973)
    1.35; 0.85   (0, 25°C, shake flask-GC, Polak & Lu 1973)
    0.431*   (shake flask-GC, measured range 25149.5°C, Price 1976)
    0.615*   (vapor saturation-GC, measured range 15–35°C, Jönsson et al. 1982)
    1.103   (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)
    1.56   (calculated-activity coeff. and K_{OW}, Tewari et al. 1982b)
    0.615   (vapor saturation-partition coefficient-GC, Jönsson et al. 1982)
    0.660   (shake flask-GC, Coates et al. 1985)
    0.762*   (37.75°C, shake flask-GC, measured range 37.75–280°C, pressure range 0.0103–8.86 MPa,
        Heidmen et al. 1985)
    ln x = −343.1497 + 13862.49/(T/K) + 49.24600·ln (T/K); temp range 37.75–280°C (shake flask-GC, Heidman
        et al. 1985)
    0.884, 0.949 (20°C, shake flask-GC, Burris & MacIntyre 1986)
    1.250   (shake flask-purge and trap-GC, Coutant & Keigley 1988)
    0.71*   (recommended, temp range 0–100°C, IUPAC Solubility Data Series, Shaw 1989)
    ln x = −415.7563 + 17975.386/(T/K) + 59.55451·ln (T/K); temp range 290–400 K (eq. derived from literature
        calorimetric and solubility data, Tsonopoulos 1999)
    0.774*   (29.9°C, shake flask-solid extraction-GC/FID, measured range 29.9–183°C, Marche et al. 2003)
    ln x = −362.618 + 14904.474/(T/K) + 52.067·ln (T/K): temp range 29.9–183°C (shake flask-solid extraction-
        GC/FID measurements, Marche et al. 2003)

0.635*   (calculated-liquid-liquid equilibrium LLE data, temp range 288.2–36.1 K, Mączyński et al. 2004)

0.807   (24.9°C, generator column-GC/FID, measured range 10–45°C, Sarraute et al. 2004)

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

486.6*   (3.7°C, static-McLeod gauge, measured range –9.31 to 3.7°C, Linder 1931)

7670*   (52.972°C, ebulliometry, measured range 52.972–126.570°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.92377 – 1355.126/(209.517 + t/°C)$; temp range 52.9–126.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

1777*   (calculated-Antoine eq. regression, temp range –14 to 125.6°C, Stull 1947)

1870   (calculated from determined data, Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.92377 – 1355.126/(209.517 + t/°C)$; temp range 40–155°C (Antoine eq. for liquid state, Dreisbach 1959)

1885*   (interpolated-Antoine eq., temp range 19.2–152.1°C, Zwolinski & Wilhoit 1971

$\log (P/\text{mmHg}) = 6.92377 – 11355.126/(209.517 + t/°C)$; temp range 19.2–152.1°C (Antoine eq., Zwolinski & Wilhoit 1971)

1825   (interpolated-Antoine eq., temp range –14 to 281.4°C, Weast 1972–73)

$\log (P/\text{mmHg}) = [–0.2185 \times 9221.0/(T/K)] + 7.894018$; temp range –14 to 281.4°C (Antoine eq., Weast 1972–73)

1573*   (23.96°C, gas saturation, measured range –56.35 to 23.96°C, Carruth & Kobayashi 1973)

1885, 2060 (quoted, calculated-bp, Mackay et al. 1982)

1860   (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.04394 – 1351.938/(209.12 + t/°C)$; temp range 52.93–126.57°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

1860   (interpolated-Antoine eq., temp range 19–152°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.91868 – 1351.99/(209.15 + t/°C)$; temp range 19–152°C (Antoine eq., Dean 1985, 1992)

1870   (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.04358 – 1351.99/(209.155 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

1854, 1814, 1854 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)

1862   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04231 – 1351.491/(–64.014 + T/K)$; temp range 297–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.90115 – 2238.9/(–4.53 + T/K)$; temp range 216–278 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.16936 – 1440.32/(–52.894 + T/K)$; temp range 396–432 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.23406 – 1492.068/(–45.851 + T/K)$; temp range 428–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.66614 – 7.66614/(159.091 + T/K)$; temp range 506–569 K (Antoine eq.-V, Stephenson & Malanowski 1987)

1872*   (recommended, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 – (T_o/K)/(T/K)]\cdot\exp\{2.90150 – 2.046204 \times 10^{-3}\cdot(T/K) + 2.010759 \times 10^{-6}\cdot(T/K)^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 398.793$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 29.0948 – 3.0114 \times 10^3/(T/K) –7.2653\cdot\log (T/K) – 2.2696 \times 10^{-11}\cdot(T/K) + 1.468 \times 10^{-6}\cdot(T/K)^2$; temp range 216–569 K (vapor pressure eq., Yaws 1994)

1820*   (24.6°C, ebulliometry, measured range 291.25–409.95 K, Dejoz et al. 1996)

$\ln (P/\text{Pa}) = 13.9183 – 3114.43/[(T/K) – 63.9225]$; temp range 291–409 K (ebulliometry, Dejoz et al. 1996)

6727*   (50.43°C, comparative ebulliometry, measured range 323–563 K, data fitted to Wagner eq., Ewing & Ochoa 2003)

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.):

326800   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee)

311900, 110670 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

325300   (calculated-P/C, Mackay & Leinonen 1975; Mackay & Shiu 1990)

323200   (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; Mackay 1981)

325000   (calculated-P/C, Mackay & Shiu 1981)

355500*   (25.1°C, equilibrium cell-concentration ratio-GC, measured range 14.8–34.92°C, Jönsson et al. 1982)

180130, 253880, 344280, 458250, 595800   (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl. data, Jönsson et al. 1982)

ln $(1/K_{AW})$ = 26003.7/(T/K) + 70.571·ln (T/K) – 494.151; temp range: 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

324200   (calculated-P/C, Lyman et al. 1982)

ln (k_H/MPa) = 357.733 – 19363.1/(T/K) – 9.04865·(T/K)^2 – 49.5296·ln (T/K); maximum k_H = 7.836 × 10^4 MPa at 372.1 K (Heidman et al. 1985)

314700   (calculated-P/C, Eastcott et al. 1988)

326200   (Valsaraj 1988)

201500   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

499500   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

39213*   (27.9°C, EPICS-GC, measured range 27.9–45°C, Hansen et al. 1993)

ln $[H/(kPa·m^3/mol)]$ = –8014/(T/K) + 30.0; temp range: 27.9–45°C (EPICS-GC, Hansen et al. 1993)

297951   (EPICS-GC, Ryu & Park 1999)

21838   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 12.08 – 3263/(T/K) (summary of literature data, Staudinger & Roberts 2001)

257797   (24.9°C, calculated-P/C, Sarraute et al. 2004)

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

4.0   (calculated-π substituent const., Hansch et al. 1968; Hansch & Leo 1979)

5.29   (calculated-activity coefficient γ, Wasik et al. 1981,1982)

5.18   (generator column-GC, Tewari et al. 1982a,b)

4.0   (HPLC-k′ correlation, Coates et al. 1985)

5.24   (generator column-GC, calculated-activity coefficient γ, Schantz & Martire 1987)

5.15 ± 0.45   (recommended, Sangster 1989; 1993)

5.61   (calculated-activity coefficients, Tse & Sandler 1994)

5.18   (recommended, Hansch et al. 1995)

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

3.55*   (20.29°C, from GC-determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization: $t_{1/2}$ = 5.55 h for a water column of 1 m^2 minimum cross section of depth 1 m (Mackay & Leinonen 1975)

estimated $t_{1/2}$ ~ 3.1 h at 20°C in a river 1 m deep flowing at 1 m s^{-1} and with a wind velocity of 3 m s^{-1} (Lyman et al. 1982).

Photolysis:

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

k_{OH}*(exptl) = 6.03 × 10^{12} cm^3 mol^{-1} s^{-1}, k_{OH}(calc) = 2.35 × 10^{12} cm^3 mol^{-1} s^{-1} at 296 K, measured range 296–497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{O(3P)}$ = 1.70 × 10^{-13} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom at room temp. (Herron & Huie 1973)

k_{OH}(exptl) = 8.42 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 K, k_{OH}(calc) = 7.35 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (Darnall et al. 1978)

$k_{OH} = (9.01 \pm 0.19) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 299 ± 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{OH} = 8.80 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 312 K in smog chamber (Nolting et al. 1988)

$k_{OH}* = 8.68 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 8.68 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.81 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

$k_{OH} = 8.71 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.81 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

$k_{OH} = 8.68 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, estimated atmospheric lifetime of 16 h (Altshuller 1991)

$k_{NO3} = 1.82 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (Atkinson 1991)

$k_{OH} = 8.68 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Paulson & Seinfeld 1992)

k_{NO3}(exptl) $=1.84 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) $= 1.79 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}* = 8.71 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3}* = 1.9 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim$ 2.4–24 h for C_4H_{10} and higher paraffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction k = 8.68×10^{-12} cm^3 molecule^{-1} s^{-1} with OH radicals with an estimated lifetime of 16 h in air during summer daylight (Altshuller 1991).

Surface water: volatilization $t_{1/2}$ = 5.55 h for a water column of 1 m^2 minimum cross section of depth 1 m (Mackay & Leinonen 1975); estimated volatilization $t_{1/2}$ = 3.1 h at 20°C in a river 1 m deep flowing at 1 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982).

Ground water:

Sediment:

Soil:

Biota:

TABLE 2.1.1.1.23.1

Reported aqueous solubilities of *n*-octane at various temperatures

1.

Nelson & De Ligny 1968		Polak & Lu 1973		Price 1976		Jonsson et al. 1982	
shake flask-GC		shake flask-GC/FID		shake flask-GC		vapor saturation-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
5	1.65	0	1.35	25.0	0.431	15	0.653
15	0.89	25	0.85	40.1	0.524	20	0.628
25	1.84			69.7	0.907	25	0.615
				99.1	1.12	30	0.612
				121.3	4.62	35	0.620
				136.6	8.52		
				149.5	11.80		

TABLE 2.1.1.1.23.1 (*Continued*)

2.

Heidman et al. 1985		Shaw 1989a		Marche et al. 2003		Mączyński et al. 2004	
shake flask-GC		IUPAC "tentative" best values		shake flask-GC		calc-recommended LLE data	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
37.75	0.76	0	0.14	29.9	0.774	15	0.698
93.35	3	20	0.63	30.3	0.762	20	0.698
148.85	24	25	0.71	69.2	1.517	25	0.635
206.35	25	30	0.61	70	2.234	30	0.635
262.35	220	40	0.8	99.9	3.046	35	0.635
279.65	380	50	1	101.1	3.414	37.7	0.635
		60	1.2	124	7.806	40.1	0.952
pressures range from		70	1.5	124	9.011	69.7	4.00
0.0103 to 8.86 MPa		80	2	131	11.23	121.3	6.98
		90	2.7	131	12.25	136.6	12.06
$\Delta H_{sol}/(kJ\ mol^{-1}) = 13.3$		100	3.7	151.2	24.88	149.5	22.21
25°C		120	7.2	165.1	43.79	262.9	50.77
		140	15	165.4	43.28		
		160	22	183	84.85		

$$\ln x = A + B/T + C \cdot \ln T$$
$$T \text{ in K}$$

A	−362.618
B	14904.474
C	52.067
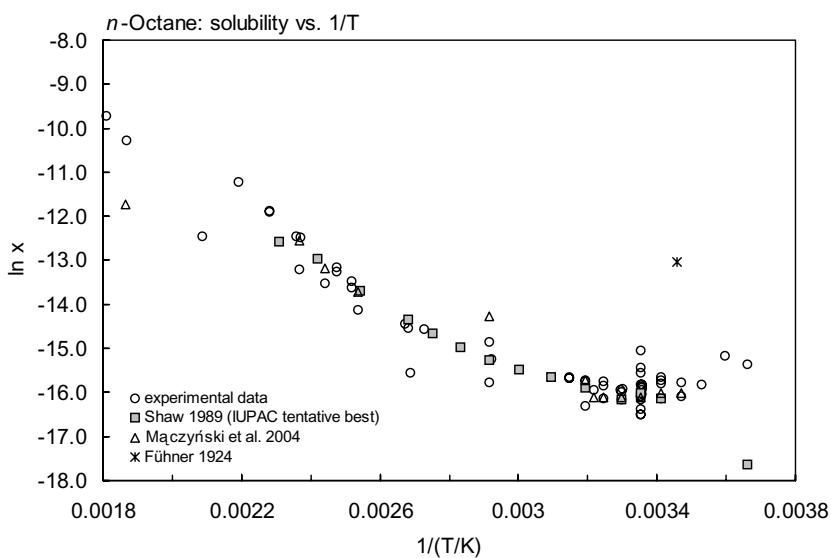
FIGURE 2.1.1.1.23.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *n*-octane.

TABLE 2.1.1.1.23.2
Reported vapor pressures of *n*-octane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(C + T/K)$	(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)		(4a)
$\ln [(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\}$	(5) - Cox eq.

1.

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−9.31	196.0	52.972	7670	−14.0	133.3	19.03	1333
−3.0	309.3	56.456	8979	8.30	666.6	39.06	2666
3.7	486.6	59.615	10314	10.2	1333	39.10	4000
		62.592	11702	31.5	2666	44.95	5333
		66.587	13823	45.1	5333	49.68	6666
		71.163	16600	53.8	7999	53.67	7999
		75.820	19918	65.7	13332	60.24	10666
		80.134	23441	83.6	26664	65.56	13332
		85.916	28952	104.0	53329	75.79	19998
		91.230	34894	125.6	101325	83.52	26664
		97.635	43326			89.813	33331
		104.233	53646	mp/°C	−56.8	95.158	39997
		111.277	66742			103.991	53329
		118.924	83695			111.204	66661
		124.319	97584			117.349	79993
		124.809	99161			122.731	93326
		125.433	100662			123.734	95992
		126.035	102386			124.715	98659
		126.570	103900			125.675	101325
		bp/°C	123.665				
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.92377			A	6.90940
		B	1355.126			B	1349.82
		C	209.517			C	209.385
		temp range: 52.9–126.6°C				bp/°C	125.675
						ΔH_V/(kJ mol^{-1})	
						at 25°C	41.49
						at bp	34.41

TABLE 2.1.1.1.23.2 *(Continued)*

2.

Carruth & Kobayashi 1973		Ruzicka & Majer 1994		Dejoz et al. 1996		Ewing & Ochoa 2003	
gas saturation		recommended		vapor-liquid equilibrium		comparative ebulliometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–56.35	2.40	194.67	0.1	18.1	1250	50.03	6727
–54.64	2.746	210.84	1.0	20.7	1450	51.811	7640
–49.92	4.40	230.53	10	24.69	1820	60.642	10766
–42.73	9.706	255.25	100	27.4	2130	67.754	14507
–35.08	20.13	287.52	1000	29.6	2410	73.195	18016
–23.06	59.33	332.03	10000	31.2	2630	79.794	23174
–13.75	127.7	398.79	101325	33.8	3020	88.950	32265
5.26	532.0	298.15	1872	36.8	3520	93.009	37123
16.41	1047			42.4	4670	99.293	45789
23.96	1573	data calc. from Cox eq.		48.6	6290	104.234	53686
		eq. 5	P/kPa	51.4	7150	110.649	65523
mp/°C	–56.81	A_0	2.90150	55.7	8690	115.266	75253
		A_1	2.046204×10^{-3}	58.9	10000	118.867	83613
eq. 1a	P/mmHg	A_2	2.010759×10^{-6}	61.4	11130	121.958	91358
A	20.3621	with reference state at		64.0	12410	125.705	101486
B	5294.36	P_o/kPa	101.325	66.7	13890	128.458	109480
		T_o/K	398.793	68.3	14820	131.853	130296
				71.8	17050	134.957	138.490
				74.9	19240		
				77.6	21330	Antoine eq. for P < 145 kPa	
				80.7	23900	in the following form	
				85.3	28330	ln P/kPa = (A–B)/(T– C)	
				90.05	34030	with	
				96.1	41180	A	13.91204
				100.5	47680	B	3110.704
				102.2	50300	C	64.086
				eq. 3(a)	kPa	for temp 323–563 K	
				A	13.9183	or pressure 6.7–2301 kPa	
				B	3114.43	data fitted to Wagner eq.	
				C	–63.925		
				for temp 291–409 K			

FIGURE 2.1.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-octane.

TABLE 2.1.1.1.23.3

Reported Henry's law constants and octanol-air partition coefficients of *n*-octane 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)		

Henry's law constant				log K_{OA}	
Jönsson et al. 1982		Hansen et al. 1993		Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
14.8	171001	27.9	39213	20.29	3.554
14.8	176031	35.0	93827	30.3	3.302
15.0	180126*	45.0	167693	40.4	3.089
20.0	253880*			50.28	2.927
20.05	259326	eq. 4	H/(kPa m³/mol)		
20.05	256596	A	30 ± 5.25		
25.0	344280*	B	8014 ± 1617		
25.1	357298				
25.1	353730				
30.0	458253*				
30.1	452643				
34.92	587452				
35.0	595804*				
* interpolated data					
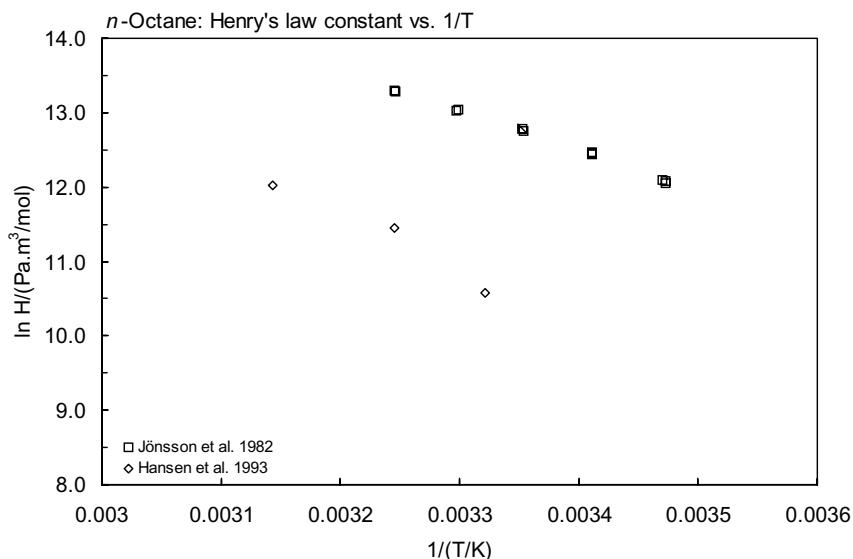
FIGURE 2.1.1.1.23.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-octane.
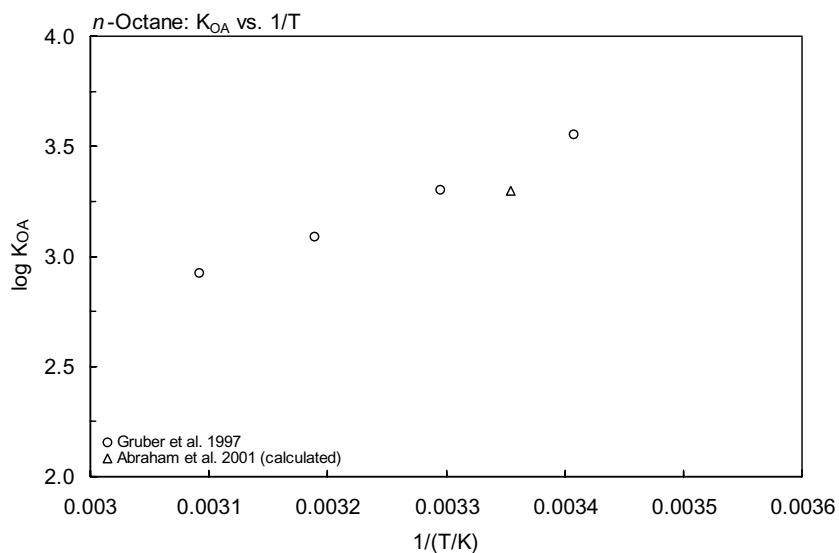
FIGURE 2.1.1.1.23.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-octane.

2.1.1.1.24   4-Methyloctane
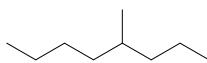
Common Name: 4-Methyloctane
Synonym:
Chemical Name: 4-methyloctane
CAS Registry No: 2216-34-4
Molecular Formula: C_9H_{20}; $CH_3(CH_2)_2CH(CH_3)(CH_2)_3CH_3$
Molecular Weight: 128.255
Melting Point (°C):
    –113.3   (Lide 2003)
Boiling Point (°C):
    142.4   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.7199, 0.7169   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
    178.2   (20°C, calculated-density)
    207.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    44.75, 36.60 (25°C, normal bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    0.115   (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    901   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.9155 – 1406.0/(206.0 + t/°C); temp range 50–165°C (Antoine eq. for liquid state, Dreisbach
        1959)
    933   (extrapolated-Antoine eq., temp range 32–170°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.90318 – 1399.12/(205.41 + t/°C); temp range 32–170°C (Antoine eq., Zwolinski & Wilhoit
        1971)
    log (P/mmHg) = 11.2012 – 2.9467 × 10^3/(T/K) + 1.2133·log (T/K) – 1.4423 × 10^{-2}·(T/K) + 9.177 × 10^{-6}·(T/K)^2;
        temp range 160–588 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
    1010000; 1000000   (calculated-P/C, recommended, Mackay & Shiu 1981)
    1007000   (selected, Mills et al. 1982)
    1007000   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Oxidation: 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:

$k_{OH} = 9.72 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 300 K (Atkinson 1989)

$k_{OH} = 9.7 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

2.1.1.1.25 n-*Nonane*
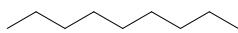
Common Name: *n*-Nonane
Synonym: nonane
Chemical Name: *n*-nonane
CAS Registry No: 111-84-2
Molecular Formula: C_9H_{20}; $CH_3(CH_2)_7CH_3$
Molecular Weight: 128.255
Melting Point (°C):
     –53.46   (Lide 2003)
Boiling Point (°C):
     150.82   (Lide 2003)
Density (g/cm³ at 20°C):
     0.7176, 0.7138   (20°C, 25°C, Dreisbach 1959)
     0.7177, 0.7138   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
     178.7, 179.7   (20°C, 25°C, calculated-density)
     207.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     44.442, 36.915   (25°C, bp, Riddick et al. 1986)
     46.55   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     15.468   (Dreisbach 1959; Riddick et al. 1986)
     6.28, 15.38   (–55.95, –53.45°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     99.2, 100.5   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
     data at other temperatures designated * are compiled at the end of this section.):
     0.220   (shake flask-GC, McAuliffe 1969;)
     0.098   (Baker 1967)
     0.071   (shake flask-GC, Krasnoshchekova & Gubertritis 1973)
     0.122*   (shake flask-GC, measured range 25–136.6°C, Price 1976)
     0.289, 0.272 (15, 20°C, vapor saturation-GC, Jönsson et al. 1982)
     0.219   (shake flask-GC, Coates et al. 1985)
     1.70*   (tentative best value, temp range 20–130°C, IUPAC Solubility Data Series, Shaw 1989)
     ln x = –433.434 + 18767.82/(T/K) + 61.940·ln (T/K); temp range 290–400 K (eq. derived from lit. calorimetric
          and solubility data, Tsonopoulos 1999)
     0.135, 0.477   (25, 100.1°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
     temperatures designated * are compiled at the end of this section.):
     6349*   (70.127°C, ebulliometry, measured range 70.127–151.764°C, Willingham et al. 1945)
     log (P/mmHg) = 6.94495 – 1435.158/(202.331 + t/°C); temp range 70.1–151.8°C (Antoine eq. from exptl. data,
          ebulliometry-manometer, Willingham et al. 1945)
     623*   (calculated-Antoine eq. regression, temp range 1.4–149.5°C, Stull 1947)
     6405*   (70.343°C, ebulliometry-manometer, measured range 70.343–151.786°C, Forziati et al. 1949)
     log (P/mmHg) = 6.93513 – 1428.811/(201.619 + t/°C); temp range 70.343–151.786°C (Antoine eq., ebulliome-
          try-manometer measurements, Forziati et al. 1949)
     580   (extrapolated-Antoine eq., Dreisbach 1959)
     log (P/mmHg) = 6.93513 – 1428.811/(201.619 + t/°C); temp range 60–185°C (Antoine eq. for liquid state,
          Dreisbach 1959)

571* (extrapolated-Antoine eq., temp range 39.32–178.48°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.93513 – 1428.811/(201.619 + t/°C); temp range 39.32–178.48°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 10456.9/(T/K)] + 8.332532; temp range 2.4–149.5°C (Antoine eq., Weast 1972–73)

404.0* (20.99°C, gas saturation, measured range –53.49 to 34.59°C, Carruth & Kobayashi 1973)

570, 713 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.0628 – 1430.638/(201.827 + t/°C), temp range: 70.434–151.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 6.0847 – 1439.2/(205.962 + t/°C), temp range: 66.61–147.86°C (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)

571 (extrapolated-Antoine eq., temp range 39–179°C, Dean 1985, 1992)

log (P/mmHg) = 6.93893 – 1431.82/(202.01 + t/°C); temp range 39–179°C (Antoine eq., Dean 1985, 1992)

570 (lit. average, Riddick et al. 1986)

log (P/kPa) = 6.06383 – 1431.82/(202.011 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

517; 571 (extrapolated-Antoine eq.-I; interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.0593 – 1429.46/(–71.33 + T/K); temp range 344–426 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.17855 – 2523.8/(T/K); temp range 219–308 K (Antoine eq.-II, Stephenson & Malanowski 1987)

580.7* (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{2.94690 – 2.061933 × 10^{-3}·(T/K) + 1.903683 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 423.932 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 8.8817 – 2.8042 × 10^3/(T/K) + 1.5262·log (T/K) – 1.0464 × 10^{-2}·(T/K) + 5.7972 × 10^{-6}·(T/K)^2; temp range 220–596 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.):

601000, 748000, 333000; 500000 (calculated-P/C values, recommended, Mackay & Shiu 1981)

147400*, 372820 (14.8, 20.05°C, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)

173520, 348200 (15, 20°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)

ln (1/K_{AW}) = 28259/(T/K) + 76.183·ln (T/K) – 524.13; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

41950* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm m^3/mol)] = –0.1847 + 202.1/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

599600 (calculated-P/C, Eastcott et al. 1988)

601000 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

459668 (EPICS-GC, Ryu & Park 1999)

42164 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 1.104 + 39/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

4.51 (estimated-HPLC-k′ correlation, Coates et al. 1985)

5.65 ± 0.60 (recommended, Sangster 1989)

5.42 (recommended, Sangster 1993)

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

Bioconcentration Factor,

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{OH} = (10.7 \pm 0.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 299 $\pm$ 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{OH} = 10.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 312 K in smog chamber (Nolting et al. 1988)

$k_{OH} = 1.02 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 1.02 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K, $k_{NO3} = 2.39 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

$k_{OH} = 1.02 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} estimated atmospheric lifetime of 14 h (Altshuller 1991)

$k_{OH} = 1.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K, $k_{NO3} = 2.30 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

$k_{NO3} = 2.41 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 $\pm$ 2 K (Atkinson 1991)

k_{NO3}(exptl) = (1.92, 2.59) $\times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) = 2.47 $\times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 $\pm$ 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 10.0 $\times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 2.3 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric t$_{1/2}$ ~ 2.4–24 h for C_4H_{10} and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); photooxidation reaction rate constant of 1.02×10^{-11} cm^3 molecule^{-1} s^{-1} with OH radical with an estimated lifetime τ = 14 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.25.1
Reported aqueous solubilities of *n*-nonane at various temperatures

Price 1976		Jonsson et al. 1982		Shaw 1989a	
shake flask-GC		vapor saturation-GC		IUPAC "tentative" best	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
25.0	0.122	15	0.289	20	0.29
69.7	0.309	20	0.272	25	0.17
99.1	0.420			30	0.14
121.3	1.70			40	0.17
136.6	5.07			50	0.22
				60	0.26
				70	0.31
				80	0.34
				90	0.37
				100	0.42
				110	0.80
				120	1.60
				130	3.20

.
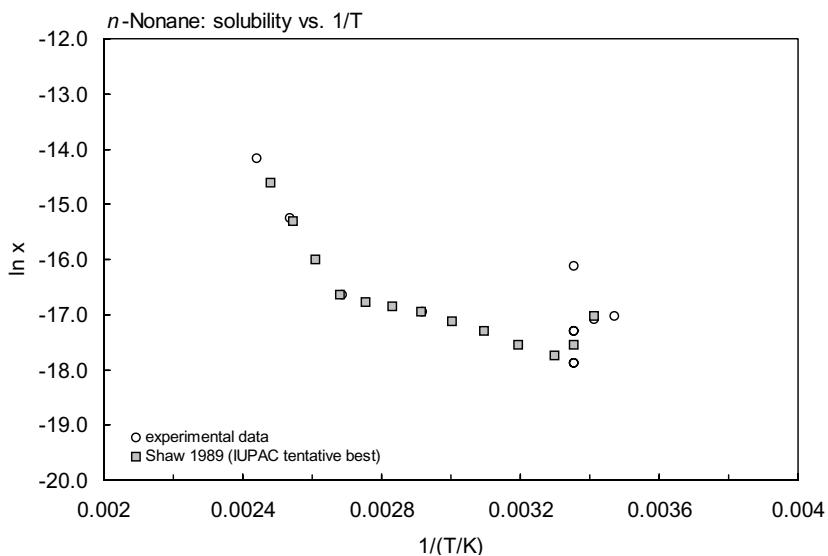
FIGURE 2.1.1.1.25.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *n*-nonane.

TABLE 2.1.1.1.25.2

Reported vapor pressures of *n*-nonane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$
$$\log P = A - B/(C + t/°C) \quad (2) \qquad \ln P = A - B/(C + t/°C) \quad (2a)$$
$$\log P = A - B/(C + T/K) \quad (3)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$
$$\ln [(P/kPa)/(P_0/kPa)] = [1 - (T_c/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\} \quad (5) \text{ - Cox eq.}$$

1.

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
ebulliometry-manometer		summary of literature data		ebulliometry-manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.127	6349	2.4	133.3	70.343	6405	39.06	1333
74.388	7650	26.3	666.6	74.546	7697	51.93	2666
78.097	8955	38.0	1333	78.219	8995	60.12	4000
81.458	10294	51.0	2666	81.548	10335	66.25	5333
84.582	11687	65.6	5333	84.658	11724	71.216	6666
88.801	13822	74.1	7999	88.864	13847	75.409	7999
93.610	16611	86.0	13332	93.601	16639	82.293	10666
98.491	19913	104.7	26664	98.545	19949	87.873	13332
103.047	23451	126.8	53329	103.072	23479	98.593	19998
109.115	28952	149.5	101325	109.136	28984	106.694	26664
114.684	34892			114.712	34.930	113.284	33331
121.399	43319	mp/°C	−53.7	121.433	43366	118.882	39997
128.329	53653			128.357	53703	128.131	53329
136.721	66757			135.741	66801	135.680	66661
143.738	83721			143.751	83755	142.110	79993
149.394	97609			149.409	97652	147.741	93326

(Continued)

TABLE 2.1.1.1.25.2 *(Continued)*

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
ebulliometry-manometer		summary of literature data		ebulliometry-manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
150.002	99207			150.017	99241	148.790	95992
150.565	100833			150.579	100734	149.816	98659
151.195	102401			151.222	102467	150.321	101325
151.764	103921			151.786	104006		
						eq. 2	P/mmHg
bp/°C	150.796			bp/°C	150.798	A	6.93440
						B	1508.75
eq. 2	P/mmHg			eq. 2	P/mmHg	C	195.374
A	6.94445			A	6.93513	bp/°C	150.821
B	1435.158			B	1428.811	ΔH_V/(kJ mol^{-1})	
C	202.331			C	201.619	at 25°C	36.92
temp range: 70.1–151.8°C				temp range: 70.3–151.8°C		at bp	46.44

2.

Carruth & Kobayashi 1973		Ruzicka & Majer 1994	
gas saturation		recommended	
t/°C	P/Pa	T/K	P/Pa
–53.49	0.7586	209.23	0.1
–49.4	0.825	226.30	1.0
–48.26	0.925	247,08	10
–36.32	3.240	273.13	100
–27.45	7.866	307.09	1000
–9.97	37.33	353.86	10000
2.60	100.4	423.392	101325
20.99	404.0	298.15	580.7
26.9	602.6		
34.59	722.6	data calc. from Cox eq.	
		eq. 5	P/kPa
mp/°C	–53.7	A_0	2.94690
		A_1	2.051933×10^{-3}
eq. 1a	P/mmHg	A_2	1.903683×10^{-6}
A	20.8468	with reference state at	
B	–5811.26	P_o/kPa	101.325
		T_o/K	423.392
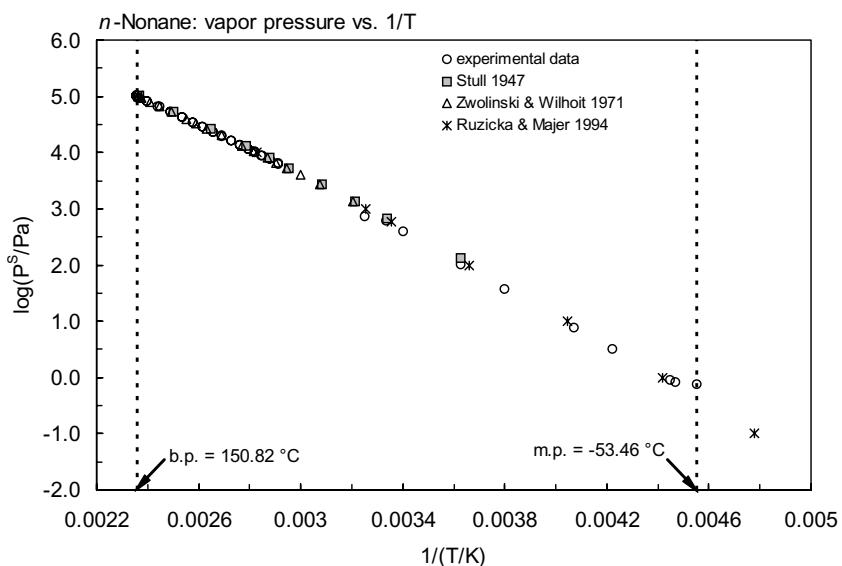
FIGURE 2.1.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-nonane.

TABLE 2.1.1.1.25.3
Reported Henry's law constants of *n*-nonane at various temperatures and temperature dependence equations

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

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

Jönsson et al. 1982		Ashworth et al. 1988	
equilibrium cell-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
14.8	244287	10	40530
14.8	221668	15	50257
15.0	237196	20	33640
20.0	348179	25	41949
20.05	369343	30	47116
20.05	363831		
		eq. 4a	H/(atm m³/mol)
		A	−0.1847
		B	202.1
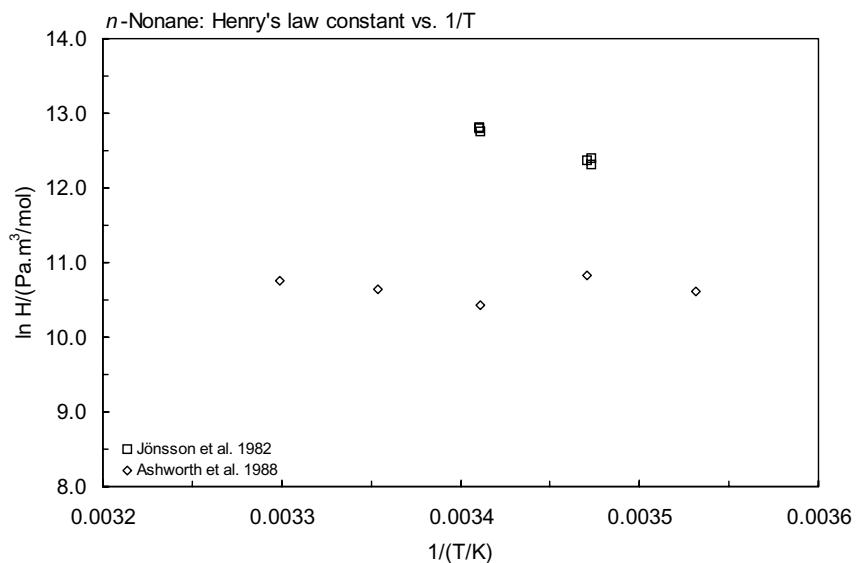
FIGURE 2.1.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-nonane.

2.1.1.1.26 n-*Decane*
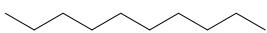
Common Name: *n*-Decane
Synonym: decane
Chemical Name: *n*-decane
CAS Registry No: 124-18-5
Molecular Formula: $C_{10}H_{22}$; $CH_3(CH_2)_8CH_3$
Molecular Weight: 142.282
Melting Point (°C):
    –29.6   (Lide 2003)
Boiling Point (°C):
    174.15   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.7301, 0.7273 (20°C, 25°C, Dreisbach 1959)
    0.7301, 0.7264 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
    194.9, 195.9 (20°C, 25°C, calculated-density)
    229.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    51.367, 31.279 (25°C, bp, Riddick et al. 1986)
    51.42   (209.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    28.72   (Dreisbach 1959)
    28.677   (Riddick et al. 1986)
    28.7   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    117.99, 109.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    0.016   (radiotracer, Baker 1958, 1959)
    0.0198   (shake flask-GC, Franks 1966)
    0.022   (Baker 1967)
    0.052   (shake flask-GC, McAuliffe 1969)
    0.0087   (shake flask-GC, Krasnoshchekova & Gubertritis 1973)
    0.182, 1.220 (shake flask-headspace-GC, Mackay et al. 1975)
    0.0029   (shake flask-refractometer, Becke & Quitzsch 1977)
    0.0524   (shake flask-GC, Coates et al. 1985)
    0.02, 0.015 (20°C, 25°C, tentative best values, IUPAC Solubility Data Series, Shaw 1989)
    0.0277, 0.0261 (20°C, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    62.66*   (8.50ºC, static-McLeod gauge, measured range –3.80 to 8.50ºC, Linder 1931)
    7649*   (94.481ºC, ebulliometry, measured range 94.481–175.121ºC, Willingham et al. 1945)
    log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t/°C); temp range 94.6–175.1°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
    238*   (calculated-Antoine eq. regression, temp range 17.1–173°C, Stull 1947)
    182   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t/°C); temp range 75–210°C (Antoine eq. for liquid state, Dreisbach 1959)
    180*   (extrapolated-Antoine eq., temp range 57.7–202.9°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t/°C); temp range 57.7–202.9°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 10912.0/(T/K)] + 8.248089; temp range 17.1–173°C (Antoine eq., Weast 1972–73)

86.53*   (16.74°C, gas saturation, measured range –29.65 to 37.45°C, Carruth & Kobayashi 1973)

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

log (P/kPa) = 6.08321 – 1504.405/(194.831 + t/°C); temp range 94.48–175.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

173   (extrapolated-Antoine eq., temp range 58–203°C, Dean 1985, 1992)

log (P/mmHg) = 6.94365 – 1495.17/(193.86 + t/°C); temp range 58–203°C (Antoine eq., Dean 1985, 1992)

180*   (24.941°C, gas saturation, measured temp range 298.091–347.887 K, Allemand et al. 1986)

170   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.55216 – 1594.49/(126.36 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

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

log (P_L/kPa) = 6.80914 – 1900.343/(–47.319 + T/K); temp range 252–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.09206 – 1510.415/(–77.646 + T/K); temp range 373–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.04899 – 1482.502/(–80.635 + T/K); temp range 447–526 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 9.71412 – 6858.314/(454.63 + T/K); temp range 524–617 K (Antoine eq.IV, Stephenson & Malanowski 1987)

874.1*   (50.64°C, static-quartz pressure gauge, measured range 50.64–314.982°C, Morgan & Kobayashi 1994)

182*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{2.96690 – 1.932579 × 10^{-3}·(T/K) + 1.644626 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 447.269 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 26.5125 – 3.3584 × 10^3/(T/K) – 6.1174·log (T/K) – 3.3225 × 10^{-10}·(T/K) + 4.8554 × 10^{-7}·(T/K)^2; temp range 243–618 K (vapor pressure eq., Yaws 1994)

127.6*   (20°C, ebulliometer and inclined piston gauge, measured temp range 268–490 K. Chirico et al. 1989)

324   (liquid P_L, GC-RT correlation; Donovan 1996)

520*   (41.6°C, ebulliometry, measured range 314.75–458.45 K, Dejoz et al. 1996)

ln (P/kPa) = 13.9735 – 3441.40/[(T/K) – 79.434]; temp range 314.75–458.45 K (ebulliometry, Dejoz et al. 1996)

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

326300   (calculated-P/C, Mackay & Shiu 1975)

499500   (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; selected, Mills et al. 1982)

489400   (calculated-P/C, Mackay 1981)

700000; 500000, 108000 (recommended; calculated-P/C, Mackay & Shiu 1981)

431100   (calculated-P/C, Eastcott et al. 1988)

477870   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

5.67   (estimated-fragment const., Lyman 1982)

6.69, 5.98   (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)

5.01   (estimated, Coates et al. 1985)

6.25 ± 0.70 (recommended, Sangster 1989)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{OH} = (11.4 \pm 0.6) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 299 ± 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{OH} = 11.7 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 1.16 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990, 1991)

$k_{OH} = 11.6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K, atmospheric lifetime of 12 h during summer daylight
(Altshuller 1991)

k_{NO3}(exptl) = 2.59×10^{-16} cm³ molecule⁻¹ s⁻¹, k_{NO3}(calc) = 2.47×10^{-16} cm³ molecule⁻¹ s⁻¹ at 296 ± K (relative
rate method, Aschmann & Atkinson 1995)

k_{OH}* = 11.2×10^{-12} cm³ molecule⁻¹ s⁻¹, k_{NO3} = 2.8×10^{-16} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended,
Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for C_4H_{10} and higher paraffins for the reaction with hydroxyl radical, based on
the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant k = 1.16×10^{-11} cm³ molecule⁻¹ s⁻¹ with hydroxyl radical with an
estimated lifetime of 12 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.26.1
**Reported vapor pressures of *n*-decane 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)		
$\ln (P/P_{ref}) = [1 - (T_{ref}/T)]·\exp(a + bT + cT^2)$	(5)		

1.

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–3.80	22.0	94.481	7649	17.1	133.3	57.6	1333
0.20	28.0	98.352	8954	42.5	666.6	71.06	2666
0.50	30.66	101.859	10292	55.4	1333	79.61	4000
8.50	62.66	105.118	11686	69.1	2666	86.02	5333
		109.526	13812	84.6	5333	91.20	6666
		114.540	16609	94.6	7999	95.576	7999
		119.640	19913	108.0	13332	102.759	10666
		124.372	23451	127.8	26664	108.579	13332
		130.690	28951	149.9	53329	119.759	19998
		136.490	34892	173.0	101325	128.203	26664

(Continued)

TABLE 2.1.1.1.26.1 (*Continued*)

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		143.495	43318			135.071	33331
		150.718	53654	mp/°C	−29.7	140.903	39997
		158.419	66757			150.535	53329
		166.772	83722			158.39	66661
		172.661	97609			165.088	79993
		173.295	99206			170.947	93326
		173.882	100701			172.039	95992
		174.538	102401			173.106	98659
		175.121	103921			174.152	101325
		bp/°C	174.123			eq. 2	P/mmHg
						A	6.95375
		eq. 2	P/mmHg			B	1508.75
		A	6.95367			C	193.374
		B	1501.268			bp/°C	174.152
		C	194.480			ΔH_V/(kJ mol^{-1})	
		temp range: 94.5–175.1°C				at 25°C	51.37
						at bp	39.28

2.

Carruth & Kobayashi 1973		Allemand et al. 1986		Chirico et al. 1989			
gas saturation		gas saturation		ebulliometry		inclined piston gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−29.65	1.72	24.941	180.0	100.086	9596	−5.002	17.0
−21.84	3.20	30.022	253.3	103.317	10897	−0.002	26.4
−18.68	4.586	35.019	352.0	106.561	12348	9.994	59.9
−9.54	10.60	40.005	481.3	109.82	13961	19.999	127.6
4.35	33.20	45.002	650.6	113.09	15752	30.001	256.1
16.74	86.53	50.006	874.6	116.373	17737	34.999	355.0
31.45	186.7	55.001	1161	119.67	19933	40.0	486.3
37.45	205.3	59.996	1520	126.299	25023	44.0	657.8
		64.916	1969	132.983	31177	50.0	879.9
mp/°C	−29.71	70.049	2545	139.716	39565	60.006	1523.8
		74.737	3190	146.502	47375	80.002	2536.1
eq. 1a	P/mmHg			153.399	57817	75.001	3227.1
A	20.8865			160.227	70120		
B	6170.32			167.167	84533		
				174.157	101325	Cox eq.	
				181.199	120790	eq. 5a	P/kPa
				188.291	143250	P_{ref}/kPa	101.325
				195.43	169920	T_{ref}/K	447.307
				202.622	198490	a	2.96081
				209.859	232020	$10^3 b$/K^{-1}	−1.90111
				217.142	270020	$10^6 c$/K^{-2}	1.60359
						temp range: 268–490 K	

TABLE 2.1.1.1.26.1 (*Continued*)

3.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994		Dejoz et al. 1996			
static-quartz pressure gauge		recommended		vapor-liquid equilibrium			
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50.64	874.1	222.67	0.1	41.6	520	144.1	44090
59.933	1509	240.65	1.0	45.2	650	146.7	47640
79.938	4050	262.50	10	49.5	840	149.3	51420
99.970	9562	289.84	100	55.2	1170	151.2	54380
119.981	20150	325.64	1000	60.1	1520	153.4	57920
119.971	20154	374.25	10000	69.1	2410	156.5	63220
139.972	38892	447.27	101325	75.8	3330	159.3	69330
159.973	69695	298.15	182.0	84.2	4900	162.3	74190
179.974	117250			93.1	7200	165.5	80890
199.976	187250	Cox eq.		97.9	8760	168.4	87350
219.976	285770	eq. 5	P/kPa	100.7	9820	174.6	102460
239.979	.420380	P_{ref}/kPa	101.325	103.5	10970	178.9	114160
259.979	598790	T_{ref}/K	447.27	105.9	12020	182.7	125370
279.98	830150	a	2.96690	108.3	13180	185.3	133470
299.98	1125900	$10^3 b$/K^{-1}	−1.932579	110.	14250		
314.982	1395000	$10^6 c$/K^{-2}	1.644626	113.3	15870	eq. 3(a)	P/kPa
				117.1	18200	A	13.9735
data fitted to Wagner eq.				121.8	21470	B	3441.40
				126.6	25280	C	−79.434
				129.4	27750	temp range 315–458 K	
				133.4	31600		
				137.2	35660		
				141.9	41250		
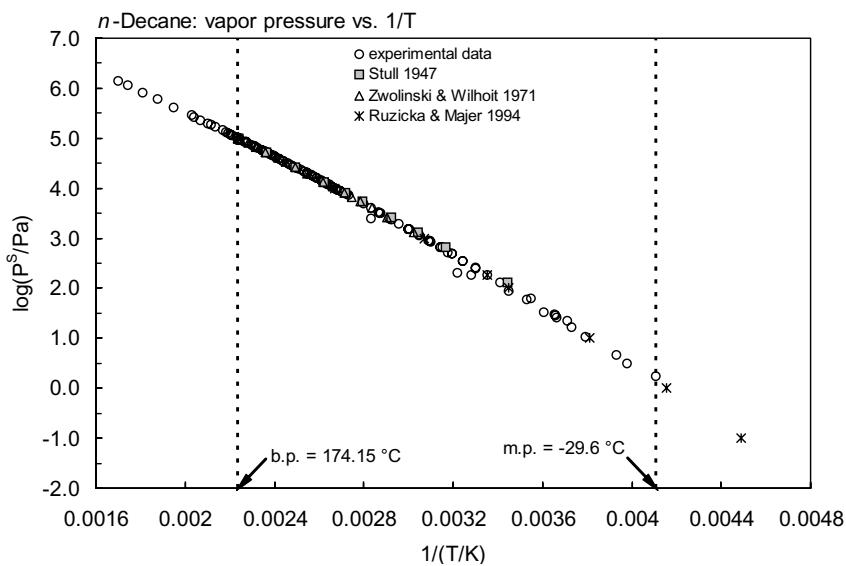
FIGURE 2.1.1.1.26.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-decane.

2.1.1.1.27   n-*Undecane*
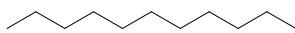
Common Name: *n*-Undecane
Synonym: undecane
Chemical Name: *n*-undecane
CAS Registry No: 1120-21-4
Molecular Formula: $C_{11}H_{24}$; $CH_3(CH_2)_9CH_3$
Molecular Weight: 156.309
Melting Point (°C):
    –25.5   (Lide 2003)
Boiling Point (°C):
    195.9   (Lide 2003)
Density (g/cm³ at 20°C):
    0.74024, 0.73652   (20°C, 25°C, Camin & Rossini 1955)
    0.7402, 0.7366   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    211.2   (20°C, calculated-density)
    251.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    56.5, 41.524 (25°C, bp, Dreisbach 1959)
    56.58   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.86, 22.18, 29.03   (–36.55, –25.55°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    118.6, 119.1   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.0044   (shake flask-GC, McAuliffe 1969)
    0.0036   (shake flask-GC, Krashoshhchekova & Gubertritis 1973)
    0.0040   ("best" value, IUPAC Solubility Data Series, Shaw 1989)
    0.0042   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    133.3*   (31.4°C, summary of literature data, temp range 31.4–194.5°C, Stull 1947)
    log (P/mmHg) = 6.97674 – 1572.477/(188.022 + t/°C); temp range 105.4–197.3°C (Antoine eq., ebulliometry-
        manometer measurement, Camin & Rossini 1955)
    57.18   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.97674 – 1572.477/(188.022 + t/°C); temp range 98–258°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    52.20*   (extrapolated-Antoine eq., temp range 75.1–225.8°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.97220 – 1569.57/(187.700 + t/°C); temp range 75.1–225.8°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 11481.7/(T/K)] + 8.260477; temp range 31.4–194.5°C (Antoine eq., Weast 1972–73)
    52.5   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.12013 – 1572.031/(188.062 + t/°C); temp range 104.5–197.3°C (Antoine eq. from reported exptl.
        data of Camin & Rossini 1955, Boublik et al. 1984)
    log (P/mmHg) = 6.97220 – 1569.57/(187.70 + t/°C); temp range 75–226°C (Antoine eq., Dean 1985, 1992)
    54.8   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.10154 – 1572.411/(–85.128 + T/K); temp range 278–470 K (Antoine eq., Stephenson &
        Malanowski 1987)
    56.89*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P$_o$/kPa)] = [1 – (T$_o$/K)/(T/K)]·exp{3.02771 – 2.045579 × 10^{-3}·(T/K) + 1.712658 × 10^{-6}·(T/K)^2}; reference state at P$_o$ = 101.325 kPa, T$_o$ = 469.042 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 82.9230 – 5.6085 × 10^3/(T/K) – 23.7327·log (T/K) + 1.0469 × 10^{-2}·(T/K) + 7.087 × 10^{-13}·(T/K)^2; temp range 248–639 K (vapor pressure eq., Yaws 1994)

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

185000   (calculated-P/C, Mackay & Shiu 1981)

185390   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

6.94   (estimated-HPLC/MS, Burkhard et al. 1985)

6.51   (calculated-fragment const., Burkhard et al. 1985)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

Oxidation: 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$_{OH}$ = 13.7 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in a smog chamber (Nolting et al. 1988)

k$_{OH}$ = 1.32 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k$_{OH}$ = 1.29 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.1.1.27.1

Reported vapor pressures of *n*-undecane 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)		
ln (P/P$_{ref}$) = [1 – (T$_{ref}$/T)]·exp(a + bT + cT^2)	(5) - Cox eq.		

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
31.4	133.3	104.58	5540	75.1	1333	236.04	0.1
58.4	666.6	110.952	8287	89.06	2666	254.71	1.0
72.2	1333	115.522	8337	97.93	4000	277.39	10
86.3	2666	118.963	9358	104.58	5333	305.75	100
103.1	5333	122.607	10954	109.95	6666	342.64	1000
113.9	7999	127.467	13104	114.486	7999	393.33	10000
126.8	13332	132.757	15837	121.934	10666	469.04	101325

(Continued)

TABLE 2.1.1.1.27.1 (*Continued*)

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
148.0	26664	138.713	19448	127.969	13332	298.15	56.89
170.6	53329	143.585	22889	139.559	19998		
194.5	101325	150.437	28550	148.312	26664	Cox eq.	
		156.841	34826	155.431	33331	eq. 5	P/kPa
mp/°C		164.039	43031	161.475	39997	P_{ref}/kPa	101.325
		171.724	53780	171.458	53329	T_{ref}/K	469.64
		179.802	67077	179.603	66661	a	3.02711
		188.431	84053	186.537	79993	10^3b/K^{-1}	–2.045579
		194.595	98132	192.608	93326	10^6c/K^{-2}	1.712658
		195.242	101081	193.739	95992		
		196.511	102882	194.845	98659		
		197.272	104822	195.928	101325		
		bp/°C	195.890	bp/°C	195.928		
		eq. 2	P/mmHg	eq. 2	P/mmHg		
		A	6.97674	A	6.97220		
		B	1572.477	B	1569.57		
		C	188.022	C	187.700		
				ΔH_V/(kJ mol^{-1}) =			
				at 25°C	56.34		
				at bp	41.50		
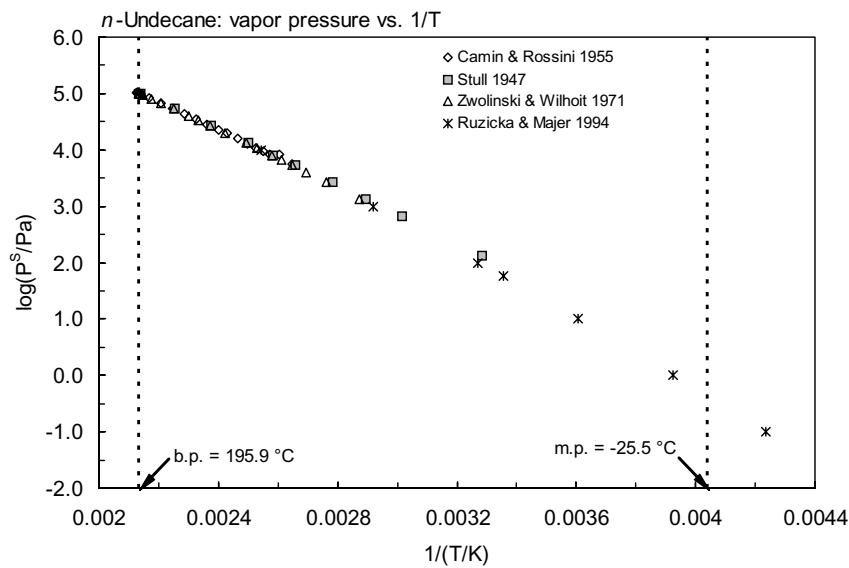
FIGURE 2.1.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-undecane.

2.1.1.1.28   n-*Dodecane*

Common Name: *n*-Dodecane
Synonym: dodecane
Chemical Name: *n*-dodecane
CAS Registry No: 112-40-3
Molecular Formula: $C_{12}H_{26}$; $CH_3(CH_2)_{10}CH_3$
Molecular Weight: 170.334
Melting Point (°C):
   –9.57   (Lide 2003)
Boiling Point (°C):
   216.32   (Lide 2003)
Density (g/cm³ at 20°C):
   0.7487, 0.7452   (20°C, 25° C, Dreisbach 1959; Riddick et al. 1986)
   0.74941   (20°C, densimeter, Dejoz et al. 1996)
Molar Volume (cm³/mol):
   227.5   (20°C, calculated-density, Stephenson & Malanowski 1987)
   273.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   61.287, 43.64   (25°, bp, Riddick et al. 1986)
   61.52   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   36.84   (Dreisbach 1959)
   35.86   (Riddick et al. 1986)
   36.82   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   139.75, 128.5   (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   0.0084   (shake flask-GC, Franks 1966)
   0.0034   (shake flask-GC, McAuliffe 1969)
   0.0037   (shake flask-GC, Sutton & Calder 1974)
   0.0037   (recommended, IUPAC Solubility Data Series, Shaw 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.):
   6365*   (126.31°C, ebulliometry, measured range 126.31–217.345°C, Willingham et al. 1945)
   log (P/mmHg) = 6.98059 – 1625.928/(180.311 + t/°C); temp range 126.4–217.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
   133.3*   (47.7°C, summary of literature data, temp range 47.7–214.5°C, Stull 1947)
   17.60   (extrapolated-Antoine eq., Dreisbach 1959)
   log (P/mmHg) = 6.98059 – 1625.928/(180.311 + t/°C); temp range 150–280°C (Antoine eq. for liquid state, Dreisbach 1959)
   15.70*   (extrapolated-Antoine eq., temp range 91.47–247.08°C, Zwolinski & Wilhoit 1971)
   7.60   (derived from compiled data, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.99795 – 1639.27/(181.835 + t/°C); temp range 91.47–247.08°C (Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = [–0.2185 × 11857.7/(T/K)] + 8.150997; temp range 47.7–345.8°C (Antoine eq., Weast 1972–73)
   15.5   (Antoine eq., Boublik et al. 1973, 1984)
   log (P/mmHg) = 6.9829 – 1627.714/(180.521 + t/°C); temp range 104.5–197.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)
   32.53   (calculated-bp, Mackay et al. 1982)

log (P/kPa) = 6.1074 – 1627.417/(180.489 + t/°C); temp range 104.5–197.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/mmHg) = 6.99795 – 1639.27/(181.84 + t/°C); temp range 91–247°C (Antoine eq., Dean 1985, 1992)

17.3*   (24.931°C, gas saturation, measured temp range 298.081–389.66 K, Allemand et al. 1986)

16.0   (lit. average, Riddick et al. 1986)

log (P/kPa) = 6.12285 – 1639.27/(181.835 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

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

log (P$_L$/kPa) = 6.62064 – 1942.122/(–65.587 + T/K); temp range 278–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.12285 – 1639.27/(–91.315 + T/K); temp range 400–492 K (Antoine eq.-II, Stephenson & Malanowski 1987)

18.40, 18.67* (25.30, 25.35°C, electronic manometry, measured range –9.27 to 98.10°C, Sasse et al. 1988)

733.8*   (79.969°C, static-differential pressure, measured range 79.969–314.982°C, Morgan & Kobayashi 1994)

18.02   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P$_o$/kPa)] = [1 – (T$_o$/K)/(T/K)]·exp{3.05854 – 2.018454 × 10^{-3}·(T/K) + 1.606849 × 10^{-6}·(T/K)^2}; reference state at P$_o$ = 101.325 kPa, T$_o$ = 489.438 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = –5.6532 –3.4698 × 10^3/(T/K) + 9.0272·log (T/K) –2.3185 × 10^{-2}·(T/K) + 1.1235 × 10^{-5}·(T/K)^2; temp range 264–658 K (vapor pressure eq., Yaws 1994)

14.1; 17.8   (liquid P$_L$, GC-RT correlation; quoted lit., Donovan 1996)

440*   (71.6°C, ebulliometry, measured range 344.25–501.55 K, Dejoz et al. 1996)

ln (P/kPa) = 14.1090 – 3781.84/[(T/K) – 90.975]; temp range 344.25–501.55 K (ebulliometry, Dejoz et al. 1996)

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

723000   (calculated-P/C, Bobra et al. 1979)

723000, 786000, 317000; 750000   (calculated-P/C values; recommended, Mackay & Shiu 1981)

721400   (selected, Mills et al. 1982)

726900   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

7.24, 7.04   (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)

6.10   (Coates et al. 1985)

6.80 ± 1.00 (recommended, Sangster 1989)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization: rate constants: k = 0.60 d^{-1}, t$_{1/2}$ = 1.1 d in spring at 8–16°C, k = 0.97 d^{-1}, t$_{1/2}$ = 0.7 d in summer at 20–22°C, k = 0.20 d^{-1}, t$_{1/2}$ = 3.6 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.377 d^{-1}, t$_{1/2}$ = 1.8 d with HgCl$_2$, and k = 1.085 d^{-1}, t$_{1/2}$ = 0.64 d without HgCl$_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

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$_{OH}$ = 15.1 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in a smog chamber (Nolting et al. 1988)

k$_{OH}$ = 14.2 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

k$_{OH}$ = 13.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

> Air: Surface water: estimated $t_{1/2}$ = 0.5 d for surface waters in case of first order reduction process (Zoeteman et al. 1980)
>
> marine mesocosm $t_{1/2}$ = 1.1 d at 8–16°C in spring, $t_{1/2}$ = 0.7 d at 20–22°C in summer and $t_{1/2}$ = 3.6 h at 3–7°C in winter when volatilization dominates, and $t_{1/2}$ = 1.8 d with $HgCl_2$ as poison, and k = 1.085 d^{-1}, $t_{1/2}$ = 0.64 d without poison in mid-September (Wakeham et al. 1983)

TABLE 2.1.1.1.28.1
Reported vapor pressures of *n*-dodecane 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)	ln P = A – B/(T/K) (1a)
ln (P/P_{ref}) = [1 – (T_{ref}/T)]·exp(a + bT + cT^2)	(5) - Cox eq.	

1.

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Allemand et al. 1986	
ebulliometry		summary of literature data		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
126.31	6365	47.7	133.3	91.47	1333	24.931	17.33
131.108	7663	75.7	666.6	105.91	2666	28.95	24.66
135.223	8971	89.9	1333	115.09	4000	29.966	26.66
138.962	10306	104.3	2666	121.96	5333	35.043	40.00
142.444	11696	121.4	5333	127.521	6666	40.023	58.13
147.152	13816	131.7	7999	132.213	7999	40.29	60.26
152.529	16611	145.5	13332	139.915	10666	45.023	84.79
157.986	19917	165.8	26664	146.153	13332	49.978	120.5
163.030	23443	188.4	53329	158.131	19998	50.0	118.8
169.814	28948	214.5	101325	167.175	26664	55.32	170.7
176.039	34896			174.527	33331	59.936	232.0
183.537	43331	mp/°C	–9.6	180.769	39997	64.936	310.6
191.255	53654			191.075	53329	69.23	409.3
199.488	66750			199.481	66661	70.093	422.6
208.417	83701			206.636	79993	74.947	558.6
214.709	97594			212.898	93326	78.83	691.9
215.303	99189			214.065	95992	80.174	745.3
216.006	100671			215.206	98659	99.87	2013
216.712	102385			216.323	101325	116.5	4258
217.345	103910						
				bp/°C	216.323		
bp/°C	216.278						
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.98059			A	6.97220		
B	1625.928			B	1639.27		
C	180.311			C	181.835		
				ΔH_V/(kJ mol^{-1}) =			
				at 25°C	61.59		
				at bp	43.64		

(Continued)

TABLE 2.1.1.1.28.1 (*Continued*)

2.

Sasse et al. 1988				Dejoz et al. 1996		Ruzicka & Majer 1994	
electronic manometry				vapor-liquid equilibrium		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–9.27	0.587	92.17	1380	71.2	440	248.34	0.1
–3.94	1.069	95.15	1599	75.6	570	267.74	1.0
0.49	1.720	98.10	1847	81.6	800	291.28	10
5.48	2.986			86.7	1040	320.68	100
5.53	2.920	eq. 2	P/mmHg	91.1	1310	358.87	1000
10.47	4.800	A	1.17283	98.2	1860	411.27	10000
15.41	6.906	B	1766.802	102	2230	489.44	101325
15.46	7.706	C	194.662	106.8	2780	298.15	18.02
20.35	12.36			111.2	3380		
20.38	12.05			118.5	4430	Cox eq.	
25.30	18.40	**Morgan & Kobayashi 1994**		122.9	5540	eq. 5	P/kPa
25.35	18.67	**static-differential pressure gauge**		126.5	6380	P_{ref}/kPa	101.325
30.27	27.60	t/°C	P/Pa	130.6	7520	T_{ref}/K	489.438
30.30	28.13			135.2	8960	a	3.05854
35.27	40.80	79.969	733.8	143	11930	10^3b/K^{-1}	–2.018454
35.30	41.33	99.970	2031	149.5	14980	10^6c/K^{-2}	1.606849
40.25	59.33	119.921	4912	154.8	17930		
40.30	60.13	139.927	10690	160.8	21810		
45.15	84.93	159.973	21248	166.1	25800		
45.22	85.86	179.974	39125	171.0	29990		
50.04	119.3	199.975	67572	175.7	34530		
50.18	121.2	219.976	110500	180.8	40060		
55.02	164.9	239.976	172410	183.3	42990		
55.12	167.3	259.979	258710	186.0	46390		
60.08	227.0	279.980	375270	189.8	51530		
60.12	230.4	299.981	528820	193.2	56510		
65.11	313.2	314.982	671130	197.6	63480		
70.09	420.2			200.0	67570		
75.08	558.4	data fitted to Wagner eq.					
76.68	612.2		see ref.	eq. 3(a)	P/kPa		
80.12	735.8			A	14.1090		
82.10	820.0			B	3781.84		
85.11	949.1			C	–90.975		
87.26	1069			temp range 345–502 K			
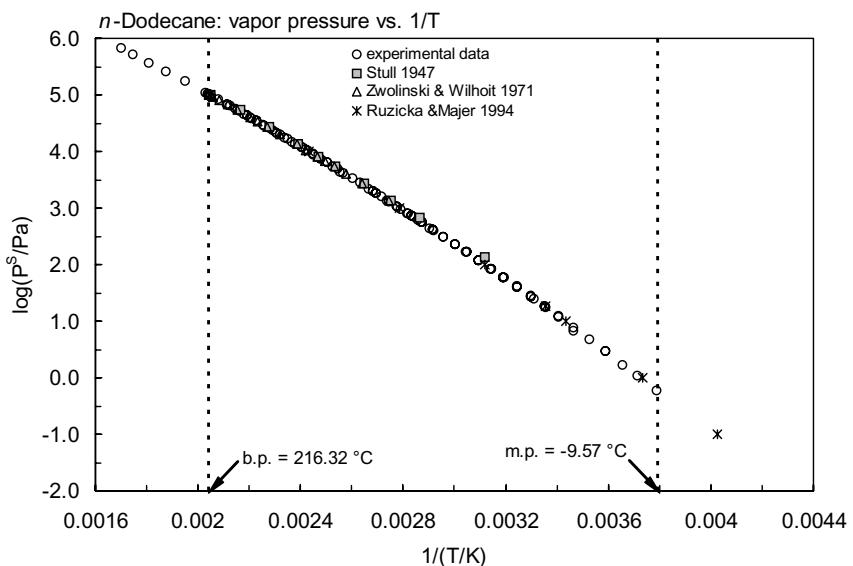
FIGURE 2.1.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-dodecane.

2.1.1.1.29 n-*Tridecane*
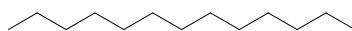
Common Name: Tridecane
Synonym:
Chemical Name: *n*-tridecane
CAS Registry No: 629-50-5
Molecular Formula: $C_{13}H_{28}$; $CH_3(CH_2)_{11}CH_3$
Molecular Weight: 184.361
Melting Point (°C):
    –5.4   (Lide 2003)
Boiling Point (°C):
    235.47   (Lide 2003)
Density (g/cm³):
    0.76522, 0.75270   (20°C, 25°C, Camin & Rossini 1955)
    0.7564, 0.7528   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    296.0   (calculated-Le Bas method at normal boiling point)
    243.7   (20°C, Stephenson & Malanowski 1987)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    66.23, 45.65 (25°C, bp, Riddick et al. 1986)
    66.68   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    28.501   (Riddick et al. 1986)
    7.66, 28.49; 36.15   (–18.15, –5.35°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    136.31, 137.8   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.00104   (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
    0.0047–0.0217   (estimated, Coates et al. 1985)
    0.06   (Riddick et al. 1986)
    0.33; 0.198   (measured; calculated molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    133.3*   (59.4°C, summary of literature data, temp range 59.4–234.0°C, Stull 1947)
    5530*   (139.3°C, ebulliometry, measured range 139.3–236.065°C, Camin & Rossini 1955)
    log (P/mmHg) = 7.00339 – 1689.093/(174.284 + t/°C); temp range 145.1–236.1°C (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)
    5.30   (extrapolated-Antoine eq., Dreisbach 1959; quoted, Riddick et al. 1986)
    log (P/mmHg) = 6.9887 – 1677.43/(172.90 + t/°C); temp range 131–302°C (Antoine eq. for liquid state, Dreisbach 1959)
    5.73*   (derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.00756 – 1690.67/(107.20 + t/°C); temp range 107.2–267.04°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 12991.3/(T/K)] + 8.481732; temp range 59.4–234°C (Antoine eq., Weast 197–73)
    4.55   (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
    log (P/mmHg = 7.00925 – 1693.684/(t/°C + 174.815); temp. range 139–236°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1973)
    log (P/kPa) = 6.13542 – 1694.624/(t/°C + 174.916); temp. range 139–236°C (Antoine eq. from reported exptl data of Camin & Rossini 1955, Boublik et al. 1984)
    log (P/mmHg) = 7.00756 – 1690.67/(174.22 + t/°C); temp range 107–267°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.13246 – 1690.67/(174.220 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 7.00756 – 1690.67/(t/°C + 174.22); temp range 107–267°C, (Antoine eq., Dean 1985; 1992)

log (P/kPa) = 6.13546 – 1690.67/(T/K – 98.93); temp range 417–511 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

5.682*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{3.10403 – 2.071819 × 10^{-3}·(T/K) + 1.61160 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 508.602 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 49.2391 – 4.9649 × 10^3/(T/K) – 13.769·log (T/K) –2.1146 × 10^{-9}·(T/K) + 2.5902 × 10^{-6}·(T/K)^2; temp range 268–676 K (vapor pressure eq., Yaws 1994)

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

233351   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

6.65   (HPLC-k′ correlation, Coates et al. 1985)

6.50; 6.05   (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = 17.5 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in a smog chamber (Nolting et al. 1988)

k_{OH} = 15.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K, 17.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 302 K (Atkinson 1989)

k_{OH} = 16.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990, 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 2.1.1.1.29.1

Reported vapor pressures of *n*-tridecane 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)		
ln (P/P_{ref}) = [1 – (T_{ref}/T)]·exp(a + bT + cT^2)	(5) - Cox eq.		

| Stull 1947 | | Camin & Rossini 1955 | | Zwolinski & Wilhoit 1971 | | Ruzicka & Majer 1994 | |
| summary of literature data | | ebulliometry | | selected values | | recommended | |
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
59.4	133.3	139.3	5530	107.2	1333	260.30	0.1
98.3	666.6	145.16	6931	122.05	2666	280.31	1.0

(Continued)

TABLE 2.1.1.1.29.1 (*Continued*)

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
104.0	1333	150.011	8326	131.48	4000	304.58	10
120.2	2666	157.603	10934	138.55	5333	335.89	100
137.7	5333	162.749	13079	144.258	6666	374.24	1000
148.2	7999	174.699	19416	149.08	7999	428.21	10000
162.5	13332	187.176	28544	156.993	10666	508.60	101325
185.0	26664	201.634	43155	163.404	13332	298.15	5.682
209.4	53329	209.788	53768	175.709	19998		
234.0	101325	218.367	67061	184.998	26664	Cox eq.	
		227.524	84040	192.55	33331	eq. 5	P/kPa
mp/°C	–6.2	234.052	85041	198.96	39997	P_{ref}/kPa	101.325
		235.316	101054	209.543	53329	T_{ref}/K	469.64
		236.065	102829	218.175	66661	a	3.10403
				225.521	79993	$10^3 b$/K^{-1}	–2.071819
				231.95	93326	$10^6 c$/K^{-2}	1.712658
				233.148	95992		
				234.319	98659		
				235.466	101325		
				25.0	5.73		
				bp/°C	235.466		
				eq. 2	P/mmHg		
				A	7.00756		
				B	1690.67		
				C	174.220		
				ΔH_V/(kJ mol^{-1}) =			
				at 25°C	66.23		
				at bp	45.65		
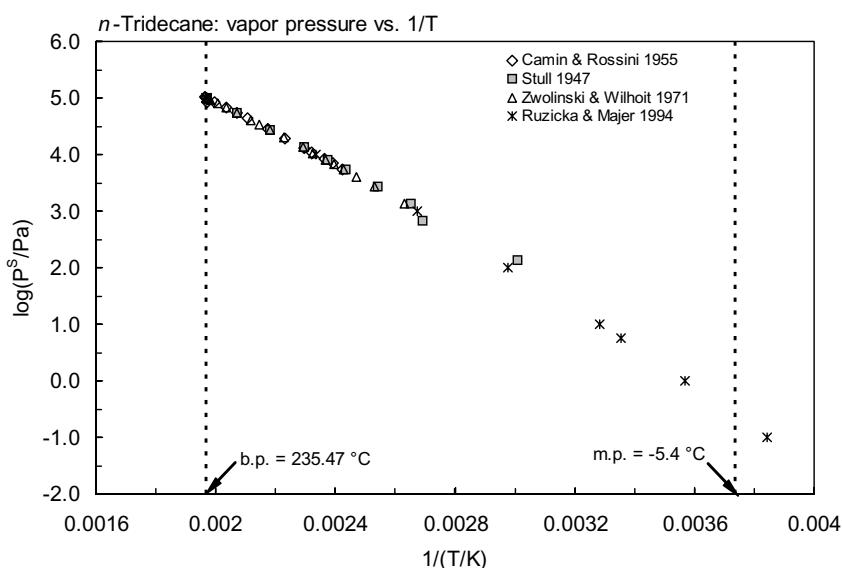
FIGURE 2.1.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tridecane.

2.1.1.1.30 n-*Tetradecane*
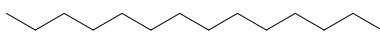
Common Name: Tetradecane
Synonym:
Chemical Name: *n*-tetradecane
CAS Registry No: 629-59-4
Molecular Formula: $C_{14}H_{30}$; $CH_3(CH_2)_{12}CH_3$
Molecular Weight: 198.388
Melting Point (°C):
    5.82   (Lide 2003)
Boiling Point (°C):
    253.58   (Lide 2003)
Density (g/cm^3):
    0.76275, 0.75917   (20°C, 25°C, Camin & Rossini 1955)
    0.7628, 0.7593   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
    260.1   (20°C, Stephenson & Malanowski 1987)
    318.2   (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    71.13, 47.73 (25°C, bp, Dreisbach 1961)
    71.73   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    45.07   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    161.54, 147.1   (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    0.0069   (shake flask-GC, Frank 1966)
    0.00655   (extrapolated, McAuliffe 1966)
    0.0022; 0.0017   (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
    0.00033   (shake flask-GC, Coates et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    133.3*   (76.4°C, summary of literature data, temp range 76.4–252.5°C, Stull 1947)
    5532*   (154.860°C, ebulliometry, measured range 154.860–254.165°C, Camin & Rossini 1955)
    log (P/mmHg) = 7.01245 – 1739.623/(167.534 + t/°C); temp range 165.9–254.2°C (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)
    1.56   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.9957 – 1725.46/(165.75 + t/°C); temp range 147–325°C (Antoine eq. for liquid state, Dreisbach 1959)
    1.27*   (Antoine eq., temp range 121.80–286.0°C, Zwolinski & Wilhoit 1971)
    1.867   (derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.01300 – 1740.88/(167.720 + t/°C); temp range 121.80–286.0°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 13750.0/(T/K)] + 8.628699; temp range 76.4–252.5°C (Antoine eq., Weast 1972–73)
    1.30   (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
    log (P/mmHg) = 7.02216 – 1747.452/(t/°C + 168.437); temp range 155–254°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1973)
    log (P/kPa) = 6.14914 – 1749.052/(t/°C + 168.611); temp range 155–254°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

log (P/mmHg) = 7.01300 – 1740.88/(t/°C + 167.72); temp. range 112–286°C (Antoine eq., Dean 1985; 1992)

72.0*   (70.01°C, gas saturation, measured temp range 343.16–394.73 K, Allemand et al. 1986)

log (P_L/kPa) = 6.62828 – 2063.84/(T/K – 77.378); temp range 313–433 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.1379 – 1740.88/(T/K – 105.43); temp range 432–529 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

442.9*   (99.926°C, static-differential pressure, measured range 99.926–314.982°C, Morgan & Kobayashi 1994)

1.804*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{3.13624 – 2.063853 × 10^{-3}·(T/K) + 1.541507 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 526.691 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 106.1056–7.3461 × 10^3/(T/K) –31.5195·log (T/K) + 1.2356 × 10^{-2}·(T/K) – 8.3955 × 10^{-13}·(T/K)^2; temp range 279–692 K (vapor pressure eq., Yaws 1994)

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

347000   (calculated-P/C, Mackay & Shiu 1981)

387000   (calculated-P/C, Eastcott et al. 1988)

114497   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

7.20   (HPLC-k′ correlation, Coates et al. 1985)

7.88, 8.10   (RP-HPLC-MS correlation, Burkhard et al. 1985)

7.00; 6.45   (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)

8.0   (recommended, Sangster 1989, 1993)

6.49   (calculated-UNIFAC, Chen et al. 1993)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = 19.3 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K in a smog chamber (Nolting et al. 1988)

k_{OH} = 19.2 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 312 K (Atkinson 1989)

k_{OH} = 19.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k_{OH} = 18.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2}$ < 15 d by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

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

Half-Lives in the Environment:

TABLE 2.1.1.1.30.1
Reported vapor pressures of *n*-tetradecane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \qquad (1)$$
$$\ln P = A - B/(T/K) \qquad (1a)$$
$$\log P = A - B/(C + t/°C) \qquad (2)$$
$$\ln P = A - B/(C + t/°C) \qquad (2a)$$
$$\log P = A - B/(C + T/K) \qquad (3)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \qquad (4)$$
$$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2) \qquad (5) \text{ - Cox eq.}$$

1.

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986	
summary of literature data		ebulliometry		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
76.4	133.3	154.860	5532	121.8	1333	70.01	71.99
106.0	666.6	165.911	6325	137.06	2666	70.45	74.53
120.7	1333	173.737	10928	146.75	4000	80.0	136.8
135.6	2666	191.234	19417	154.01	5333	91.0	262.7
152.7	5333	204.019	28546	159.881	6666	106.78	634.6
164.0	7999	218.84	43156	164.836	7999	121.58	1324
178.5	13332	236.013	67061	172.967	10666		
201.8	26664	245.408	84041	179.553	13332		
226.8	53329	252.104	98106	192.196	19998		
252.5	101325	253.401	101061	201.739	26664		
		254.165	102850	209.497	33331		
mp/°C	5.5			216.082	39997		
		bp/°C	253.516	226.953	53329		
				235.819	66661		
				243.364	79993		
				249.967	93326		
				251.197	95992		
				252.4	98659		
				253.577	101325		

(Continued)

TABLE 2.1.1.1.30.1 (*Continued*)

2.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
differential pressure gauge		recommended	
t/°C	P/Pa	T/K	P/Pa
99.926	442.9	271.60	0.1
119.936	1227	292.22	1.0
139.946	3026	317.21	10
159.956	6693	348.38	100
179.965	13526	388.82	1000
199.976	25267	444.22	10000
219.976	44274	526.69	101325
229.964	57442	298.15	1.804
239.977	73530		
249.979	93059	Cox eq.	
259.979	116500	eq. 5	P/kPa
249.979	116520	P_{ref}/kPa	101.325
279.980	177570	T_{ref}/K	526.691
299.980	261560	a	3.13624
309.982	314050	$10^3 b$/K^{-1}	−2.063853
314.982	343450	$10^6 c$/K^{-2}	1.541507

data fitted to Wagner eq.
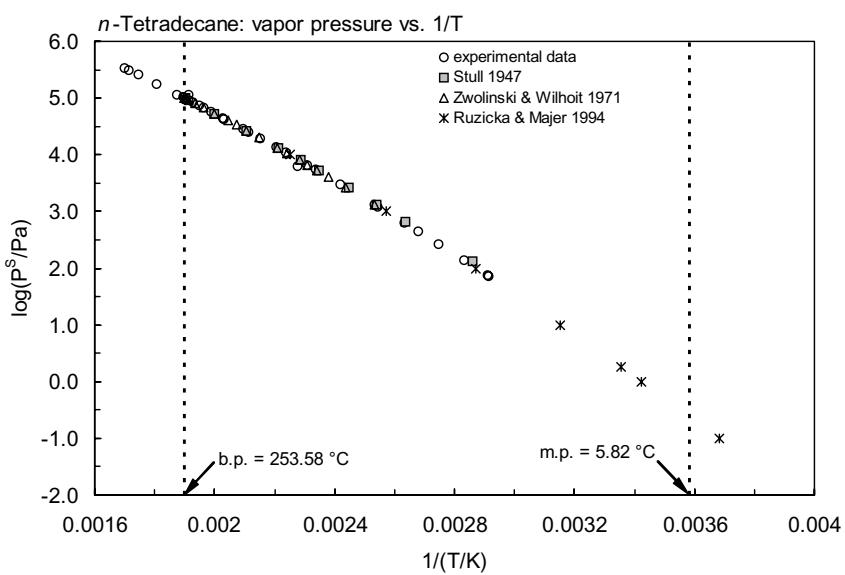
FIGURE 2.1.1.1.30.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tetradecane.

2.1.1.1.31   n-*Pentadecane*
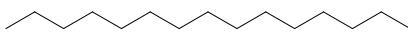
Common Name: Pentadecane
Synonym:
Chemical Name: *n*-pentadecane
CAS Registry No: 629-62-9
Molecular Formula: $C_{15}H_{32}$; $CH_3(CH_2)_{13}CH_3$
Molecular Weight: 212.415
Melting Point (°C):
    9.95   (Lide 2003)
Boiling Point (°C):
    270.6   (Camin & Rossini 1955; Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³):
    0.76830, 0.76488 (20°C, 25°C, Camin & Rossini 1955)
    0.7685, 0.7650 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    276.4   (20°C, calculated-density)
    340.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    76.16, 49.41 (25°C, bp, Dreisbach 1961)
    76.77   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.17, 34.6; 43.77 (–2.25, 9.95; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    156.02, 156.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    7.6×10^{-5} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
    0.0612; 0.0613 (measured; calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    133.3*   (91.6°C, summary of literature data, temp range 91.6–270.5°C, Stull 1947)
    5532*   (169.686°C, ebulliometry, measured range 169.686–270.449°C, Camin & Rossini 1955)
    log (P/mmHg) = 7.02445 – 1789.658/(161.291 + t/°C); temp range 169.6–270.6°C (Antoine eq., ebulliometry-
        manometer measurements, Camin & Rossini 1955)
    0.311   (extrapolated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 7.0017 – 1768.82/(158.60 + t/°C); temp range 160–338°C (Antoine eq. for liquid state, Dreisbach
        1959)
    1333*   (135.8°C, derived from compiled data, temp range 135.8–270.685°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.01359 – 1789.95/(161.380 + t/°C); temp range 135.8–303.8°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 14635.9/(T/K)] + 8.822087; temp range 91.6–270.5°C (Antoine eq., Weast 1972–73)
    0.356   (extrapolated-Antoine eq., Boublik et al. 1973)
    log P/mmHg = 7.03121 – 1797.239/(t/°C + 164.128); temp range 170–270°C (Antoine eq. from exptl. data of
        Camin & Rossini 1955, Boublik et al. 1973)
    0.359   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.15888 – 1797.239/(t/°C + 162.128); temp range 170–270.5°C (Antoine eq. derived from exptl.
        data of Camin & Rossini 1955, Boublik et al. 1984)
    log (P/mmHg) = 7.02359 – 1789.95/(161.38 + t/°C); temp range 136–304°C (Antoine eq., Dean 1985, 1992)
    15.87*   (60.0°C, gas saturation, measured temp range 60.0–136.0°C, Allemand et al. 1986)

log $(P_L/kPa) = 6.38149 - 1945.469/(T/K - 97.875)$; temp range 366–409 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.14849 - 1789.95/(T/K - 111.77)$; temp range 447–546 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

0.576*   (recommended, Ruzicka & Majer 1994)

ln $[(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{3.16144 - 2.062348 \times 10^{-3} \cdot (T/K) + 1.487263 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 543.797$ K (Cox equation, Ruzicka & Majer 1994)

log $(P/mmHg) = 116.5157 - 8.041 \times 10^3/(T/K) - 38.799 \cdot \log (T/K) - 1.3398 \times 10^{-2} \cdot (T/K) - 4.4444 \times 10^{-6} \cdot (T/K)^2$; temp range 283–707 K (vapor pressure eq., Yaws 1994)

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

48535   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

7.72   (HPLC-k′ correlation, Coates et al. 1985)

7.50; 6.78   (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization: volatilization rate constant of $k = 0.69$ d⁻¹ with a water column $t_{1/2} = 1.0$ d at 6–18°C, in spring; $k = 0.85$ d⁻¹ with a water column $t_{1/2} = 0.8$ d at 20–22°C in summer; $k = 0.16$ d⁻¹ with a water column $t_{1/2} = 4.3$ d at 3–7°C in winter for mesocosm experiment in coastal marine environment when volatilization dominates, volatilization $k = 0.343$ d⁻¹ with a water column $t_{1/2} = 2.0$ d with HgCl₂ poisoned water tank and $k = 1.241$ d⁻¹ with a water column $t_{1/2} = 0.56$ d for non-poisoned water tank in late summer (Wakeham et al. 1983).

Photolysis:

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

$k_{OH} = 22.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 22.2 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 312 K (Atkinson 1989)

$k_{OH} = 22.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)

$k_{OH} = 22.2 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (experimental); 17.87×10^{-12} cm³ molecule⁻¹ s⁻¹ (Atmospheric Oxidation Program); and 7.47×10^{-12} cm³ molecule⁻¹ s⁻¹ (Fate of Atmospheric Pollutants) for gas-phase reaction with OH radicals (Meylan & Howard 1993)

$k_{OH} = 21.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2} < 15$ d by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

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

Half-Lives in the Environment:

Surface water: water column half-lives, $t_{1/2} = 1.0$ d, 6–18°C, in spring; $t_{1/2} = 0.8$ d, 20–22°C, in summer; $t_{1/2} = 4.3$ d, 3–7°C, in winter for mesocosm experiment in coastal marine mesocosm; $t_{1/2} = 2.0$ d with HgCl poisoned water tank and $t_{1/2} = 0.56$ d for non-poisoned water tank in late summer (Wakeham et al. 1983).

TABLE 2.1.1.1.31.1

Reported vapor pressures of *n*-pentadecane at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2)$ (5) - Cox eq.

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986	
summary of literature data		ebulliometry		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
91.6	133.3	169.686	5532	135.8	1333	60.0	15.87
121.0	666.6	180.919	8325	151.41	2666	72.84	35.60
135.4	1333	188.905	10927	161.45	4000	81.53	64.13
150.2	2666	206.886	19417	168.78	5333	94.31	148.0
167.7	5333	219.982	26546	174.785	6666	111.0	394.0
178.4	7999	235.150	43159	179.859	7999	136.0	1465
194.0	13332	151.703	67061	188.185	10666		
216.1	26664	262.310	84081	194.949	13332		
242.8	53329	269.164	98106	207.872	19998	**Ruzicka & Majer 1994**	
270.5	101325	270.449	101069	217.641	26664	recommended	
				225.582	33331	T/K	P/Pa
mp/°C	10	bp/°C	270.613	232.517	39997		
				243.446	53329	282.39	0.1
				252.517	66661	303.58	1.0
				260.237	79993	329.24	10
				266.992	93326	361.22	100
				268.25	95992	402.67	1000
				269.48	98659	459.40	10000
				270.685	101325	543.80	101325
						298.15	0.576
				bp/°C	270.685		
						Cox eq.	
				eq. 2	P/mmHg	eq. 5	P/kPa
				A	7.02359	P_{ref}/kPa	101.325
				B	1789.95	T_{ref}/K	543.64
				C	161.380	a	3.16774
						$10^3 b$/K^{-1}	–2.062348
				ΔH_V/(kJ mol^{-1}) =		$10^6 c$/K^{-2}	1.487263
				at 25°C	76.15		
				at bp	49.45		
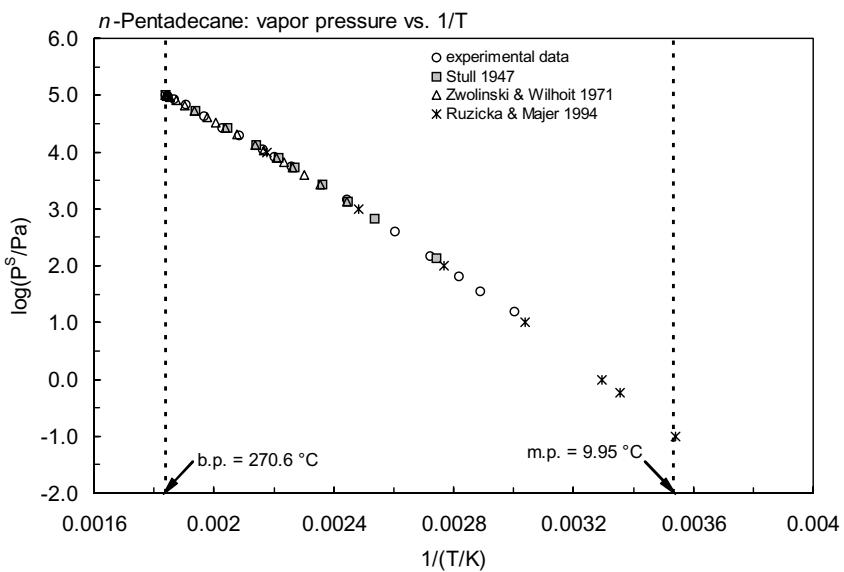
FIGURE 2.1.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-pentadecane.

2.1.1.1.32 n-*Hexadecane*

Common Name: Hexadecane
Synonym: cetane
Chemical Name: *n*-hexadecane
CAS Registry No: 544-76-3
Molecular Formula: $C_{16}H_{34}$; $CH_3(CH_2)_{14}CH_3$
Molecular Weight: 226.441
Melting Point (°C):
   18.12   (Lide 2003)
Boiling Point (°C):
   286.86   (Lide 2003)
Density (g/cm³):
   0.77344, 0.76996 (20°C, 25°C, Camin et al. 1954; Dreisbach 1959)
   0.7733   (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
   292.8   (20°C, calculated-density, Stephenson & Malanowski 1987)
   362.2   (calculated-Le Bas molar volume at normal boiling point, Eastcott et al. 1988)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   81.35   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   53.35, 51.46; 53.35 (18.15, 17.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   176.79, 165.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   6.28×10^{-3} (shake flask, Franks 1966)
   2.1×10^{-5} (extrapolated data of McAuliffe 1966, Coates et al. 1985)
   5.21×10^{-5} (extrapolated from data of McAuliffe 1996, Eastcott et al. 1988)
   9.0×10^{-4}, 4.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
   2.33×10^{-6} (calculated-TSA, Lande et al. 1985)
   0.0272   (calculated-molar volume correlation, Wang et al. 1992)
   4.95×10^{-5} (calculated-molar volume and mp., Ruelle Kesselring 1997)

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*   (105.3°C, summary of literature data, temp range 105.3–287.5°C, Stull 1947)
   6945*   (190.054°C, ebulliometry, measured range 190.054–286.704°C, Camin et al. 1954)
   13.33*   (81.0°C, static method-Hg manometer, measured range 81.0–286.0°C, Myers & Fenske 1955)
   log (P/mmHg) = 7.03044 – 1831.317/(154.528 + t/°C); temp range 190.0–286.8°C (Antoine eq., ebulliometry-
      manometer measurements, Camin et al. 1954)
   0.14   (71.87°C, calculated-Antoine eq., Dreisbach 1959)
   0.221*   (derived from compiled data, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 7.02867 – 1830.51/(154.450 + t/°C); temp range 149.18–320.7°C (Antoine eq., Zwolinski &
      Wilhoit 1971)
   log (P/mmHg) = [–0.2185 × 15405.5/(T/K)] + 8.956267; temp range 105.3–287.5°C (Antoine eq., Weast
      1972–73)
   0.092   (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
   log (P/mmHg) = 7.03519 – 1835.24/(t/°C + 154.968); temp range 188–285°C (Antoine eq. from exptl. data of
      Camin et al. 1945, Boublik et al. 1973)
   log (P/kPa) = 6.16189 – 1836.287/(t/°C + 155.125); temp range 190–287°C (Antoine eq. from exptl. data of
      Camin et al. 1954, Boublik et al. 1984)

log (P/mmHg) = 7.02867 – 1830.51/(154.45 + t/°C); temp range 149–321°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 6.77064 – 2273.168/(T/K – 80.252); temp range 323–425 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.15357 – 1830.57/(T/K – 118.7); temp range 467–563 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.02967 – 1830.51/(t/°C + 154.45); temp range 149–321°C (Antoine eq., Dean 1992)

log (P/mmHg) = 99.1091 – 7.5333 × 10³/(T/K) – 32.251·log (T/K) + 1.0453 × 10⁻²·(T/K) + 1.2328 × 10⁻¹²·(T/K)²; temp range 291–721 K (vapor pressure eq., Yaws 1994)

317.6*   (119.896°C, static-differential pressure, measured range 119.896–309.982°C, Morgan & Kobayashi 1994)

0.191*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{3.18271 – 2.002545 × 10⁻³·(T/K) + 1.384476 × 10⁻⁶·(T/K)²}; reference state at P_o = 101.325 kPa, T_o = 559.978 K (Cox equation, Ruzicka & Majer 1994)

0.190   (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant (Pa·m³/mol at 25°C):
    389000   (calculated-P/C, Eastcott et al. 1988)
    23072   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    8.25   (HPLC-k′ correlation, Coates et al. 1985)
    8.00; 7.26   (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
        k_{OH} = 25.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 312 K (Atkinson 1989)
        k_{OH} = 25.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)
        k_{OH} = 23.0 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biodegradation: microbial degradation $t_{1/2}$ < 31 d by *Pseudomonas* sp. (Setti et al. 1993)
    Biotransformation:
    Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 2.1.1.1.32.1
Reported vapor pressures of *n*-hexadecane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2)$	(5) - Cox eq.		

1.

Stull 1947		Camin et al. 1954		Myers & Fenske 1955		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		static method-Hg manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
105.3	133.3	190.054	6945	81.0	13.33	149.18	1333
135.2	666.6	193.301	8330	94.2	66.66	165.14	2666
149.8	1333	199.273	9351	105.3	133.3	175.28	4000
164.7	2666	203.437	10951	117.2	266.6	182.87	5333
181.2	5333	208.962	13098	124.9	400.0	189.00	6666
193.2	7999	215.00	15824	130.7	533.3	194.184	7999
208.5	13332	221.78	19448	135.5	666.6	202.682	10666
231.7	26664	227.336	22886	138.2	799.9	209.565	13332
258.3	53329	235.145	28558	145.0	1067	222.774	19998
287.5	101325	242.432	34817	150.0	1333	232.743	26664
		250.605	43171	159.5	2000	240.846	33331
mp/°C	18.5	259.336	53777	166.0	2666	247.723	39997
		268.540	67076	176.0	4000	259.074	53329
		278.333	84.065	183.6	5333	268.33	66661
		285.337	98168	189.7	6666	276.205	79993
		286.704	101325	194.3	7999	283.097	93326
				202.6	10666	284.38	95992
		bp/°C	286.792	209.8	13332	285.635	98659
				222.3	19998	286.864	101325
		eq. 2	P/mmHg	232.2	26664	25.0	0.221
		A	7.03044	245.8	39997	bp/°C	286.854
		B	1831.317	258.0	53329		
		C	154.528	267.0	66661	eq. 2	P/mmHg
				274.5	79993	A	7.02867
				282.2	93326	B	1830.51
				286.0	101325	C	154.450
						$\Delta H_V/(kJ\ mol^{-1}) =$	
						at 25°C	81.09
						at bp	51.21

(Continued)

TABLE 2.1.1.1.32.1 (*Continued*)

2.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
static method pressure gauge		recommended	
t/°C	P/Pa	T/K	P/Pa
119.896	317.6	292.41	0.1
129.903	541.2	314.20	1.0
139.909	886.1	340.55	10
149.916	1408	373.36	100
159.929	2172	415.82	1000
169.929	3273	473.84	10000
179.935	4810	559.98	101325
189.943	6912	298.15	0.191
199.976	9774		
209.956	13530	Cox eq.	
219.976	18418	eq. 5	P/kPa
229.969	24691	P_{ref}/kPa	101.325
239.977	32600	T_{ref}/K	469.64
249.979	42464	a	3.18271
259.979	54642	$10^3 b$/K^{-1}	–2.002545
269.979	69438	$10^6 c$/K^{-2}	1.384476
279.980	87294		
289.980	108620		
299.980	133940		
309.982	163530		
data fitted to Wagner eq.			
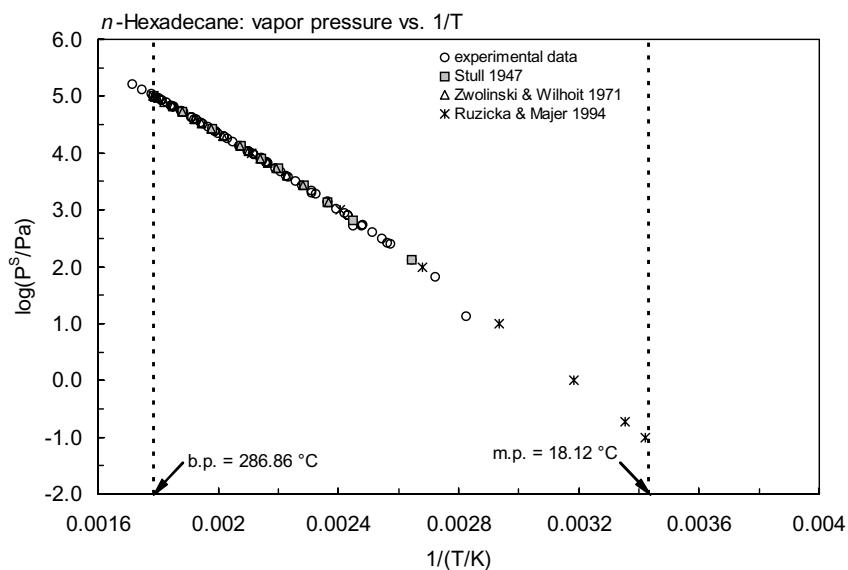
FIGURE 2.1.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexadecane.

2.1.1.1.33 n-*Heptadecane*
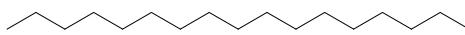
Common Name: Heptadecane
Synonym:
Chemical Name: *n*-heptadecane
CAS Registry No: 629-78-7
Molecular Formula: $C_{17}H_{36}$; $CH_3(CH_2)_{15}CH_3$
Molecular Weight: 240.468
Melting Point (°C):
    22   (Lide 2003)
Boiling Point (°C):
    302   (Lide 2003)
Density (g/cm³):
    0.7780, 0.7745 (20°C, 25°C, Dreisbach 1959)
    0.7780   (Weast 1982–83)
Molar Volume (cm³/mol):
    384.8   (calculated-Le Bas method at normal boiling point)
    309.1   (20°C, calculated-density)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    61.65, 53.12 (25°C, bp, Dreisbach 1961)
    86.47   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    10.96, 40.17; 51.13 (1.15, 21.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    174.61, 175.1   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al.1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    5.5×10^{-6} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
    0.0014   (reported as –log S (mol/L) = 7.24, calculated-molar volume, Wang et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    1467*   (163.5°C, temp range 163.5–303.0°C, Krafft 1882; quoted, Boublik et al. 1984)
    133.3*   (115.0°C, summary of literature data, temp range 115.0–303.0°C, Stull 1947)
    log (P/mmHg) = 7.0115 – 1847.82/(145.52 + t/°C); temp range 188–374°C (Antoine eq. for liquid state, Dreisbach 1959)
    0.0253*   (derived from compiled data, temp range 160.9–337°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.0143 – 1865.1/(149.20 + t/°C); temp range 160.9–337°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 15608.5/(T/K)] + 8.847487; temp range 115–303°C (Antoine eq., Weast 1972–73)
    0.030   (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
    log (P/mmHg) = 6.97509 – 1851.699/(t/°C + 149.263); temp range 164–303°C (Antoine eq., Boublik et al. 1973)
    log (P/kPa) = 6.09247 – 1845.726/(t/°C + 148.633); temp range 164–303°C (Antoine eq., Boublik et al. 1984)
    log (P/mmHg) = 7.10143 – 1865.1/(t/°C + 149.20); temp range 161–337°C (Antoine eq., Dean 1985, 1992)
    0.015   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 11.1197 – 4757.087/(T/K); temp range 289–320 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.1392 – 1865.1/(T/K – 123.95); temp range 488–577 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
    0.06148*   (recommended, Ruzicka & Majer 1994)
    ln [(P/kPa)/(P_o/kPa)] = $[1 – (T_o/K)/(T/K)]$_exp{3.21826 – 2.036553 × 10^{-3}·(T/K) + 1.383899 × 10^{-6}·(T/K)²}; reference state at P_o = 101.325 kPa, T_o = 575.375 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 173.4039 –1.0943 × 10⁴/(T/K) –59.212·log (T/K) + 2.0705 × 10⁻²·(T/K) –1.3433 × 10⁻¹²·(T/K)²;
    temp range 295–733 K (vapor pressure eq., Yaws 1994)
0.0627   (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant (Pa m³/mol at 25°C):
    5415   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    8.92; 9.69   (estimated-RP-HPLC-MS; calculated-CLOGP, Burkhard et al. 1985)
    8.79   (HPLC-k′ correlation, Coates et al. 1985)
    8.50; 7.68   (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:
    Volatilization: volatilization k =1.23 d⁻¹ with a water column $t_{1/2}$ = 0.6 d at 6–18°C in spring; k = 0.79 d⁻¹ with
        a water column $t_{1/2}$ = 0.9 d at 20–22°C in summer; k = 0.14 d⁻¹ with a water column $t_{1/2}$ = 5.0 d at 3–7°C in
        winter for mesocosm experiments in coastal marine environment; volatilization k = 0.359 d⁻¹ with a water
        column $t_{1/2}$ = 1.9 d with HgCl poisoned water tank and k = 1.362 d⁻¹ with a water column $t_{1/2}$ = 0.51 d for
        non-poisoned water tank in late summer (Wakeham et al. 1983).
    Photolysis:
    Oxidation:
    Hydrolysis:
    Biodegradation: microbial degradation $t_{1/2}$ < 31 d by *Pseudomonas sp.* (Setti et al. 1993)
    Biotransformation:
    Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
    Surface water: water column $t_{1/2}$ = 0.6 d at 6–18°C, in spring; $t_{1/2}$ = 0.9 d at 20–22°C, in summer; $t_{1/2}$ = 5.0 d at
        3–7°C, in winter for mesocosm experiment in coastal marine environment; $t_{1/2}$ = 1.9 d with HgCl poisoned
        water tank and $t_{1/2}$ = 0.51 d for non-poisoned water tank in late summer (Wakeham et al. 1983).

TABLE 2.1.1.1.33.1
Reported vapor pressures of *n*-heptadecane 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)
ln (P/P_ref) = [1 – (T_ref/T)]·exp(a + bT + cT²)   (5) - Cox eq.

| Stull 1947 | | Krafft 1882 | | Zwolinski & Wilhoit 1971 | | Ruzicka & Majer 1994 | |
| summary of literature data | | in Boublik et al. 1984 | | selected values | | recommended | |
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
115.0	133.3	163.5	1467	160.9	1333	302.38	0.1
145.2	666.6	170.0	2000	177.3	2666	324.64	1.0
160.0	1333	187.5	4000	187.6	4000	351.56	10
177.7	2666	201.5	6666	195.4	5333	385.06	100
195.8	5333	223.0	13332	201.7	6666	428.4	1000

TABLE 2.1.1.1.33.1 (*Continued*)

Stull 1947		Krafft 1882		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		in Boublik et al. 1984		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
207.3	7999	303.0	101325	207	7999	487.59	10000
223.0	13332			215.7	10666	575.38	101325
247.8	26664	bp/°C	303.003	222.76	13332	298.15	0.06148
274.5	53329			236.30	19998		
303.0	101325			246.50	26664	Cox eq.	
				254.82	33331	eq. 5	P/kPa
mp/°C	22.5			261.87	39997	P_{ref}/kPa	101.325
				273.51	53329	T_{ref}/K	469.64
				283.0	66661	a	3.21826
				291.08	79993	$10^3 b$/K^{-1}	−2.036553
				298.14	93326	$10^6 c$/K^{-2}	1.383899
				299.47	95992		
				300.76	98659		
				302.02	101325		
				bp/°C	302.02		
				eq. 2	P/mmHg		
				A	7.0143		
				B	1865.10		
				C	149.20		
				ΔH_V/(kJ mol^{-1}) =			
				at 25°C	86.20		
				at bp	52.89		
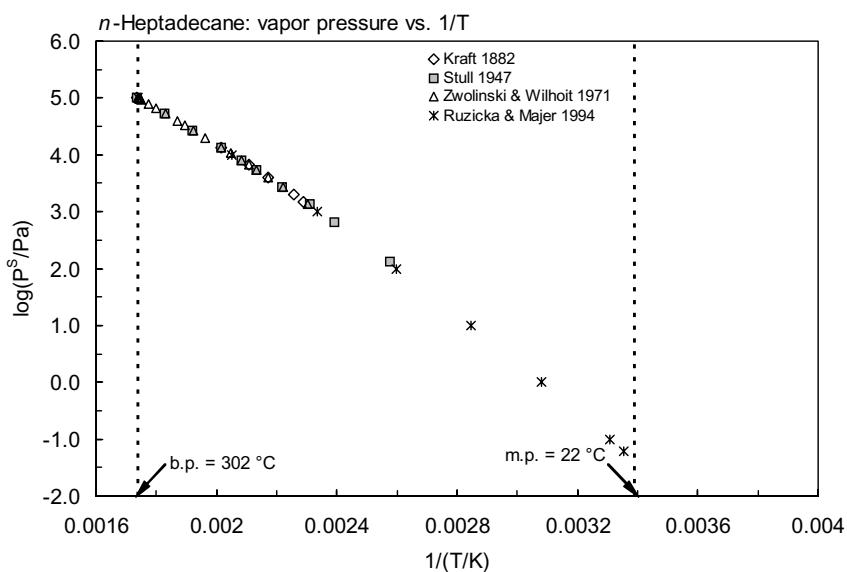
FIGURE 2.1.1.1.33.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-heptadecane.

2.1.1.1.34   n-*Octadecane*
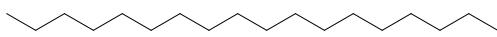
Common Name: Octadecane
Synonym:
Chemical Name: *n*-octadecane
CAS Registry No: 543-45-3
Molecular Formula: $C_{18}H_{38}$; $CH_3(CH_2)_{16}CH_3$
Molecular Weight: 254.495
Melting Point (°C):
    28.2   (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
    316.3   (Lide 2003)
Density (g/cm^3):
    0.7819, 0.7785   (20°C, 25°C, Dreisbach 1959)
    0.7768   (Weast 1982–83)
Molar Volume (cm^3/mol):
    325.5   (20°C, calculated-density)
    407.0   (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
Enthalpy of vaporization, ΔH_V (kJ/mol):
    90.824, 54.84   (25°C, bp, Dreisbach 1959)
    91.6   (25°C, Piacente et al. 1994)
    91.44   (298.15K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    61.384   (Dreisbach 1959)
    61.13   (28°C, Piacente et al. 1994)
    61.5   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    204.6, 184.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.930 (mp at 28.2°C)

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

    7.75×10^{-3} (Baker 1959)
    2.1×10^{-3}; 8.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
    1.40×10^{-6} (extrapolated from data of McAuliffe 1966, Coates et al. 1988)
    4.05×10^{-6} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)

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*   (119.6°C, summary of literature data, temp range 119.6–317.0°C, Stull 1947)
    26.66*   (102.4°C, static method-Hg manometer, measured range 102.4–313°C, Myers & Fenske 1955)
    log (P/mmHg) = 7.0156 – 1883.73/(139.46 + t/°C); temp range 201–387°C (Antoine eq. for liquid state, Dreisbach 1959)
    1333*   (172.3°C, derived from compiled data, temp range 172.3–316.3°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.0022 – 1894.3/(143.3 + t/°C); temp range 172.3–352°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 15447.0/(T/K)] + 8.619864; temp range 119.6–317°C (Antoine eq., Weast 1972–73)
    0.013   (extrapolated-Antoine eq., Boublik et al. 1973)
    log (P/mmHg) = 7.14067 – 2012.745/(t/°C + 155.492); temp range 174–317°C (Antoine eq., Boublik et al. 1973)
    0.0259   (liquid P_L, extrapolated-Antoine eq., Macknick & Prausnitz 1979)
    0.220*   (45.0°C, gas saturation, measured range 45.0–88.10°C, Macknick & Prausnitz 1979)
    ln (P_L/mmHg) = 25.548 – 10165/(T/K); temp range 45–88.1°C (Antoine eq. on exptl. data, gas saturation, liquid state, Macknick & Prausnitz 1979)

0.0133   (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.27065 - 2016.983/(t/°C + 155.924)$; temp range 174–317°C (Antoine eq., Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.0022 - 1894.3/(143.30 + t/°C)$; temp range 172–352°C (Antoine eq., Dean 1985, 1992)

1.15*   (62.04°C, gas saturation, measured temp range 335.19–439.82 K, Allemand et al. 1986)

0.0261   (extrapolated-Antoine eq.-I, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 10.18833 - 4404.095/(T/\text{K})$; temp range 310–361 K Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1392 - 1894.3/(T/\text{K} - 129.85)$; temp range 501–550 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 7.0022 - 1894.3/(t/°C + 143.30)$; temp range 172–352°C (Antoine eq., Dean 1992)

256.6*   (139.919°C, static-differential pressure, measured range 139.919–314.982°C, Morgan & Kobayashi 1994)

0.02007*   (recommended, temp range 396–500 K, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/\text{K})/(T/\text{K})] \cdot \exp\{3.24741 - 2.048039 \times 10^{-3} \cdot (T/\text{K}) + 1.362445 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 590.023$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = -15.0772 - 4.8702 \times 10^3/(T/\text{K}) + 14.501 \cdot \log (T/\text{K}) - 3.1625 \times 10^{-2} \cdot (T/\text{K}) + 1.3478 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 273–591 K (vapor pressure eq., Yaws 1994)

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

1013   (15°C, Wakeham et al. 1986)

622200   (calculated-P/C, Eastcott et al. 1988)

893   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

9.32   (HPLC-k′ correlation, Coates et al. 1985)

9.00; 8.13   (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.90   (K_{OM}, Wakeham et al. 1986)

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

Volatilization: volatilization rate constant $k_v = 0.03$ d^{-1}, microcosm exptl. (Wakeham et al. 1986).

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: degradation rate constant of about 0.66 d^{-1} in a microcosm expt. (Wakeham et al. 1986); microbial degradation $t_{1/2} < 31$ d by *Pseudomonas sp.* (Setti et al. 1993).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: an estimated $t_{1/2} = 1.5$ d in Rhine River for a first order reduction process in river water (Zoeteman et al. 1980)

$t_{1/2} \sim 23$ d in a seawater microcosm experiment (Wakeham et al. 1986).

TABLE 2.1.1.1.34.1
Reported vapor pressures of *n*-octadecane at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2)$ (5) - Cox eq.

1.

Stull 1947		Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979	
summary of literature data		ebulliometry		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
119.6	133.3	102.4	26.66	172.3	1333	45.0	0.220
152.1	666.6	115.9	66.66	189.0	2666	51.45	0.400
169.6	1333	127.0	133.3	199.6	4000	54.5	0.568
187.5	2666	139.6	266.6	207.5	5333	54.85	0.591
207.4	5333	147.0	400.0	213.9	6666	59.85	0.935
219.7	7999	153.3	533.3	219.3	7999	65.60	1.529
236.0	13332	157.7	666.6	228.2	10666	71.25	2.493
260.6	26664	161.8	799.9	234.39	13332	80.85	5.826
288.0	53329	167.7	1067	249.21	19998	84.10	7.148
317.0	101325	172.8	1333	259.64	26664	88.10	9.719
		182.8	2000	268.12	33331		
mp/°C	28	189.6	2666	275.32	39997	eq. 1a	P/mmHg
		199.9	4000	287.2	53329	A	25.548
		208.0	5333	296.9	66661	B	10165
		214.3	6666	305.2	79993		
		219.5	7999	312.4	93326		
		228.5	10666	313.7	95992		
		235.7	13332	315.0	98659		
		249.0	19998	316.3	101325		
		259.2	26664				
		273.8	39997	bp/°C	316.3		
		286.0	53329				
		294.7	66661	eq. 2	P/mmHg		
		302	79993	A	7.0022		
		308	93326	B	1894.3		
		313	101325	C	143.30		
				$\Delta H_V/(kJ\ mol^{-1}) =$			
				at 25°C	90.8		
				at bp	54.48		

TABLE 2.1.1.1.34.1 (*Continued*)

2.

Allemand et al. 1986		Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
gas saturation		vapor-liquid equilibrium		recommended	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
62.04	1.1506	139.919	256.6	311.88	0.1
71.39	2.680	149.924	443.6	334.61	1.0
84.0	6.599	159.93	729.4	362.08	10
88.0	9.479	169.936	1148	396.24	100
97.0	18.40	179.974	1761	440.41	1000
100.4	22.00	189.948	2637	500.70	10000
110.0	43.86	199.976	3870	590.02	101325
124.21	106.1	209.976	5566	298.15	0.02007
130.0	152.0	219.976	7834		
140.0	264.0	229.977	10835	Cox eq.	
166.67	995.9	239.970	14744	eq. 5	P/kPa
		254.979	22736	P_{ref}/kPa	101.325
		254.979	27300	T_{ref}/K	469.64
		264.979	34026	a	3.24741
		284.980	49559	$10^3 b$/K^{-1}	–2.048039
		299.98	70490	$10^6 c$/K^{-2}	1.362445
		314.982	98240		
		data fitted to Wagner eq.			
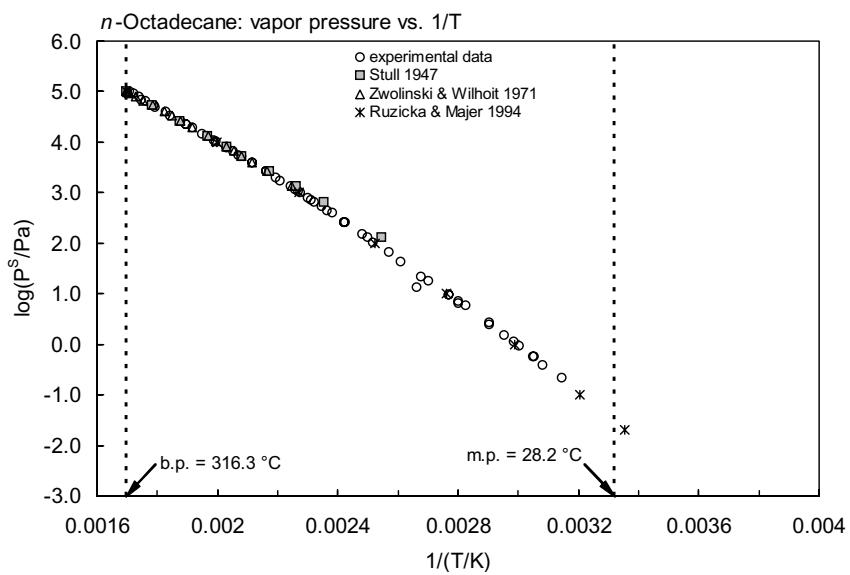
FIGURE 2.1.1.1.34.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-octadecane.

2.1.1.1.35   n-*Eicosane*

Common Name: Eicosane
Synonym: didecyl
Chemical Name: *n*-eicosane
CAS Registry No: 112-95-8
Molecular Formula: $C_{20}H_{42}$; $CH_3(CH_2)_{18}CH_3$
Molecular Weight: 282.547
Melting Point (°C):
    36.6   (Lide 2003)
Boiling Point (°C):
    334.8   (Chirico et al. 1989)
Density (g/cm³):
    0.7887, 0.7853   (20°C, 25°C, Dreisbach 1959)
    0.7886   (Weast 1982–83)
Molar Volume (cm³/mol):
    451.4   (calculated-Le Bas molar volume at normal boiling point)
    358.2   (20°C, calculated-density)
    358   (Wang et al. 1992)
Enthalpy of vaporization, ΔH_V (kJ/mol):
    63.93; 64.35   (exptl., calculated, Macknick & Prausnitz 1979b)
    100.9; 110   (25, 94°C, Piacente et al. 1994)
    101.81   (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    69.875   (Dreisbach 1959)
    69.5   (Piacente et al. 1994)
    67.8   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    219.6, 203.1 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.769 (mp at 36.6°C)

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

    1.9×10^{-3}, 8.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
    1.10×10^{-7} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
    3.11×10^{-7} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    13.33*   (121.9°C, static method-Hg manometer, measured range 121.9–342.0°C, Myers & Fenske 1955)
    log (P/mmHg) = 7.0225 – 1948.7/(127.8 + t/°C), temp range: 224–417°C, (Antoine eq. for liquid state, Dreisbach 1959)
    1333*   (198.3°C, derived from compiled data, temp range 198.3–343.8°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.1522 – 2032.7/(132.1 + t/°C); temp range:198.3–379°C (Antoine eq., Zwolinski & Wilhoit 1971)
    0.41*   (71.5°C, P_L, gas saturation-IR, Macknick & Prausnitz 1979)
    ln (P_L/mmHg) = 26.849 – 11230/(T/K); temp range: 71.15–107.3°C, (Antoine eq., gas saturation, liquid state, Macknick & Prausnitz 1979)
    log (P_L/kPa) = 10.77373 – 4872.63/(T/K); temp range: 344–380 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.2771 – 2032.7/(T/K – 141.05); temp range 528–620 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
    0.201*   (79.97°C, pressure gauge, measured range 90.07–194.21°C, Sasse et al. 1988)

log (P/mmHg) = 7.95834 – 2665.762/(t/°C + 167.047); (Antoine eq. derived from exptl. data, liquid phase, pressure gauge measurement, Sasse et al. 1988)

15.6*   (115°C, inclined piston measurement, temp range 115–215°C, Chirico et al. 1989)

ln (P/kPa) = 19.36 – 9083/(T/K); temp range 406–472 K (transpiration method, Piacente et al. 1991)

ln (P/kPa) = 22.53 – 10649/(T/K); temp range 345–393 K (torsion method, Piacente et al. 1991)

ln (P/kPa) = 18.10 – 7889/[(T/K) + 32]; temp range 315–472 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)

log (P/mmHg) = 7.1522 – 2032.1/(t/°C + 132.10); temp range 198–379°C (Antoine eq., Dean 1992)

0.32*, 0.641 (74, 78°C, torsion-effusion method, measured range 74–115°C, Piacente et al. 1994)

log (P/kPa) = 13.37 – 5785/(T/K); temp range 351–384 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 12.96 – 5709/(T/K); temp range 347–389 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.16 – 5747/(T/K); temp range ~ 347–388 K, ΔH_V = 110 kJ mol^{-1} (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)

0.002091*   (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T_o/K)/(T/K)]·exp{3.31181 – 2.102218 × 10^{-3}·(T/K) + 1.348780 × 10^{-6}·(T/K)^2}; reference state at P_o = 101.325 kPa, T_o = 617.415 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 19.4193 – 5.8699 × 10^3/(T/K) – 44.282·log (T/K) – 1.2606 × 10^{-2}·(T/K) + 5.2241 × 10^{-6}·(T/K)^2; temp range 310–767 K (vapor pressure eq., Yaws 1994)

0.00209*   (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant (Pa·m^3/mol):

198300   (calculated-P/C, Eastcott et al. 1988)

32.73   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

10.39   (HPLC-k′ correlation, Coates et al. 1985)

10.0; 8.92   (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Biodegradation: microbial degradation $t_{1/2}$ < 31 d by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.35.1

Reported vapor pressures of eicosane 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)	
$\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT)^2$	(5)	

1.

Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979		Sasse et al. 1988	
Hg manometer		selected values		gas saturation		electronic manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
121.9	13.33	198.3	1333	71.15	0.4106	90.07	2.333
136.5	66.6	215.3	2666	79.90	0.973	90.12	2.360
148.6	133.3	326.1	4000	86.70	1.693	100.17	5.526
162.0	266.6	234.1	5333	90.35	2.333	100.17	5.266
170.0	400.0	240.7	6666	94.50	3.266	110.16	11.49
176.7	533.3	246.1	7999	102.95	6.719	110.16	11.43
182.0	666.6	255.15	10666	107.30	9.133	120.06	22.53
185.7	799.9	262.41	13332			120.10	22.80
192.6	1067	276.39	19998			130.11	43.20
198.0	1333	286.91	26664	eq. 1a	P/mmHg	130.13	43.73
208.8	2000	295.45	33331	A	26.849	139.99	80.66
215.7	2666	302.70	39997	B	11230	140.03	79.86
226.4	4000	314.60	53329			149.88	141.61
234.7	5333	324.4	66661			149.97	144.9
241.3	6666	332.6	79993			159.73	243.7
246.5	7999	339.8	93326			159.83	245.7
255.7	10666	341.2	95992			169.61	404.2
262.5	13332	342.5	98659			169.68	410.6
276.1	19998	343.8	101325			179.49	657.3
286.4	26664					189.25	1025
300.2	39997	bp/°C	343.8			194.21	1266
312.0	53329						
320.0	66661	eq. 2	P/mmHg			eq. 2	P/mmHg
327.0	79993	A	7.1522			A	7.99897
333.0	93326	B	2032.7			B	2067.622
342.0	101325	C	132.1			C	177.32
		$\Delta H_V/(kJ\ mol^{-1}) =$					
		at 25°C	100.8				
		at bp	57.49				

TABLE 2.1.1.1.35.1 (*Continued*)

2.

Chirico et al. 1989				Piacente et al. 1991			
ebulliometry		inclined piston gauge		transpiration method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				1st set		2nd set data	
250.795	9596	115.0	15.6	150.85	114.8	124.85	23.99
254.896	10897	120.001	21.9	155.85	138.0	129.85	43.65
259.013	12348	125.001	30.7	160.35	182.0	134.35	37.15
263.144	13961	130.0	42.3	163.85	218.8	149.35	97.72
267.291	15752	135.0	58.3	166.85	275.4	152.85	123.0
271.454	17737	140.0	78.7	169.85	309.0	154.35	134.9
275.628	19933	150.0	139.9	171.85	371.5	156.35	147.9
284.032	25023	170.0	397.9	175.85	416.9	159.35	177.8
292.481	31177	180.0	641.9	177.85	537.0	165.85	218.8
300.985	38565	190.0	1007.7	180.35	537.0	169.85	281.8
309.540	46375	200.0	1539.6	182.85	537.0	172.35	275.4
318.146	57817	210.0	2300.3	185.85	645.7	174.35	354.8
326.761	70120	215.0	2789.0	188.35	831.8	176.35	426.6
335.416	84533			190.35	812.8	179.85	489.8
344.053	101325	Cox vapor pressure eq.		192.35	871.0	184.85	537.0
352.842	120790	eq. 5	P/kPa	193.85	912.0	188.85	645.7
		P_{ref}/kPa	101.325	196.85	1096.5	191.85	741.3
enthalpy of vaporization:		T_{ref}/K	617.456	198.85	1175	194.35	851.1
ΔH_V/(kJ mol^{-1}) =		a	3.31018			196.35	831.8
380 K	89.07	10^3b/K^{-1}	–2.09538				
400 K	86.133	10^6c/K^{-2}	1.34198				
420 K	83.448	temp range: 388–626 K					
440 K	80.78						
460 K	78.20						
480 K	75.68						
500 K	73.21						
520 K	70.75						
540 K	68.27						
560 K	65.74						
580 K	63.12						
600 K	60.37						
620 K	57.44						

(*Continued*)

TABLE 2.1.1.1.35.1 (*Continued*)

3.

Piacente et al. 1991 (cont'd)							
transpiration (cont'd)		torsion method				Knudsen method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
3rd set data		cell B, #1		cell B, #3		cell AK	
131.35	64.57	71.85	0.575	66.35	0.3802	42	0.0288
135.35	67.61	77.85	1.148	73.85	0.7586	51	0.10
141.35	107.15	81.85	1.514	78.85	1.148	60	0.269
145.85	114.82	84.35	1.905	82.85	1.698	70	0.5888
150.35	158.49	87.85	2.455	84.85	2.089	cell AK	
157.35	194.98	90.85	3.020	87.85	2.630	70	0.741
159.85	229.09	96.85	4.169	89.85	3.388	77	1.318
162.35	257.04	97.85	5.888	91.85	3.981	83	1.738
163.85	295.12	101.85	6.761	95.85	4.786	93	4.467
166.35	281.84	104.35	8.710	97.85	6.026		
179.35	338.84	105.35	9.333	101.85	7.943		
174.35	436.52	108.35	11.48	110.35	15.14	Eq. for transpiration, torsion	
177.85	524.81	112.35	16.22	117.35	25.12	and Knudsen effusion	
183.35	707.95	112.85	17.38	117.85	25.70	eq. 3a	P/kPa
185.35	691.83	114.85	19.20	118.85	26.92	A	18.10 ± 0.23
187.85	812.83	cell B #2		cell B, #4		B	7889 ± 230
191.85	977.24	88.85	2.8184	71.35	0.5754	C	−32 ± 10
192.85	1023.3	89.85	3.388	78.35	1.148		
		90.85	3.388	82.85	1.698		
		91.85	3.802	86.85	2.291	bp /°C	343.65
Antoine eq. for transpiration		95.85	4.571	89.85	3.388	mp/°C	36.65
eq. 1a	P/kPa	96.85	4.898	104.85	10.0		
A	19.36 ± 0.46	97.35	5.129	107.85	11.48	ΔH_{fus}/(kJ mol^{−1}) = 69.882	
B	9083 ± 207	1–2.35	7.943	109.35	13.18	at 298.15 K	
		104.35	8.710	110.85	15.49	ΔH_{subl}/(kJ mol^{−1}) = 152.3	
		106.83	9.550	112.85	18.62	at 298.15 K	
		107.85	10.72	115.85	22.91		
		108.85	12.02	117.85	28.18		
		109.85	13.18	119.85	32.36		
		110.85	14.79				
		111.85	16.98	Antoine eq. for torsion			
		112.85	19.50	eq. 1a	P/kPa		
				A	22.53 ± 0.30		
				B	10649 ± 230		

TABLE 2.1.1.1.35.1 (*Continued*)

4.

| Piacente et al. 1994				Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
torsion-effusion				static pressure gauge		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
run a		run b		top-cut			
77.85	0.641	73.85	0.32	159.903	244	330.01	0.1
79.85	0.961	77.85	0.481	169.91	401.8	353.55	1.0
81.85	1.28	80.85	0.641	179.918	641.1	381.97	10
83.85	1.52	82.85	0.801	189.926	1006	417.30	100
85.85	1.84	85.85	1.28	199.934	1537	462.95	1000
88.85	2.40	88.85	1.60	199.976	1538	525.23	10000
91.85	3.36	91.85	2.40	209.976	2301	617.41	101325
93.85	4.17	94.85	3.04	219.947	3358	298.15	0.002091
94.85	4.97	97.85	4.17	229.954	4812		
98.85	6.57	100.85	4.65	239.961	6771	Cox eq.	
101.85	8.33	103.85	6.89	249.969	9359	eq. 5	P/kPa
103.85	10.40	106.85	8.65	259.979	12738	P_{ref}/kPa	101.325
107.85	15.1	112.85	14.3	269.979	17040	T_{ref}/K	617.415
110.85	19.4	114.85	17.1	284.980	25728	a	3.31181
				299.980	37745	10^3b/K^{-1}	−2.102218
eq. for run a		eq. for run b		314.982	54210	10^6c/K^{-2}	1.248780
eq. 1	P/kPa	eq. 1	P/kPa	mid-cut			
A	13.37	A	12.96	159.847	244.9		
B	5785	B	5709	169.853	401		
temp range: 351–384 K		temp range: 347–388 K		179.860	639		
				189.875	999.1		
ΔH_V/(kJ mol^{-1}) =		By weighing the slopes and		199.874	1541		
at 298.15 K	100.9	intercepts of above 2 eq.,		209.884	2302		
at 367 K	110 ± 2	selected vapor pressure eq.		219.894	3349		
		eq. 1	P/kPa	229.911	4813		
mp/°C	28	A	13.16	239.915	6773		
ΔH_{fus}/(kJ mol^{-1}) = 61.10		B	5747	249.931	9349		
				259.938	12736		
ΔH_{subl}/(kJ mol^{-1}) = 152.7		ΔH_V/(kJ mol^{-1}) = 110 ± 2		269.949	17029		
		at 367 K		279.957	22549		
				289.970	29252		
				299.970	37754		
				309.982	48080		
				data fitted to Wagner eq.			
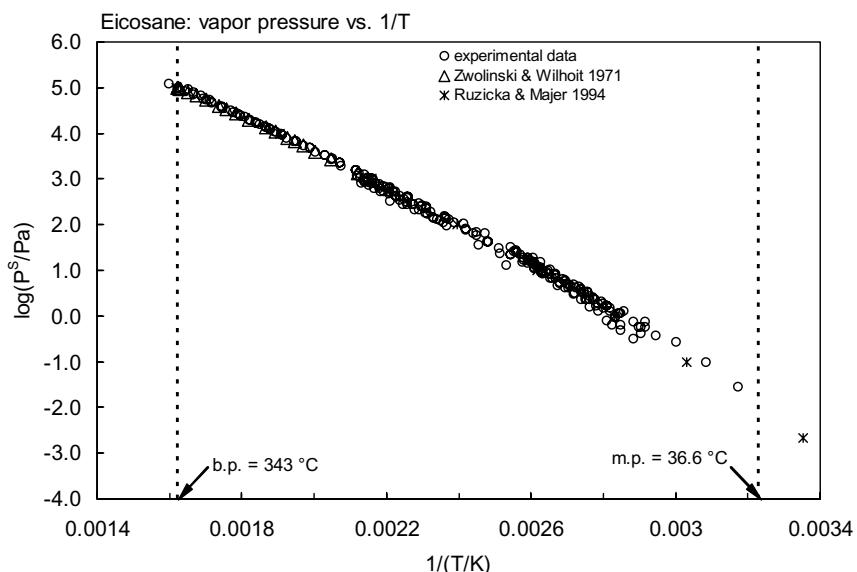
FIGURE 2.1.1.1.35.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-eicosane.

2.1.1.1.36 n-*Tetracosane*

Common Name: Tetracosane
Synonym:
Chemical Name: *n*-tetracosane
CAS Registry No: 646-31-1
Molecular Formula: $C_{24}H_{50}$; $CH_3(CH_2)_{22}CH_3$
Molecular Weight: 338.654
Melting Point (°C):
    50.4   (Lide 2003)
Boiling Point (°C):
    391.3   (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³):
    0.7991, 0.7958 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    540.2   (calculated-Le Bas method at normal boiling point)
    423.8   (20°C, calculated-density)
Enthalpy of vaporization, ΔH_V (kJ/mol):
    126   (132°C, Piacente et al. 1994)
    121.9   (calculated, Chickos & Hanshaw 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    54.9   (Dreisbach 1959; Piacente et al. 1994)
    31.3, 54.89; 86.19   (48.15, 50.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    266.79, 240.4   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.563 (mp at 50.4°C)

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

    5.8×10^{-10} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    133.3*   (183.8°C, summary of literature data, temp range 183.8–386.4°C, Stull 1947)
    $\log (P/mmHg) = 7.53923 - 2591.9/(165.1 + t/°C)$; temp range 260–500°C (Antoine eq. for liquid state, Dreisbach
        1959)
    $\log (P/mmHg) = 7.0976 - 2112.0/(109.6 + t/°C)$ (Antoine eq., Kudchadker & Zwolinski 1966)
    66.66*   (175.9°C, derived from compiled data, temp range 175.9–391.3°C, Zwolinski & Wilhoit 1971)
    $\log (P/mmHg) = 7.0976 - 2112.0/(109.6 + t/°C)$; temp range 175.9–391.3°C (Antoine eq., Zwolinski & Wilhoit
        1971)
    $\log (P/mmHg) = [-0.2185 \times 19642.5/(T/K)] + 9.408166$; temp range 183.8–386.4°C (Antoine eq., Weast
        1972–73)
    $\log (P_L/kPa) = 6.44051 - 2289.02/(T/K - 147.92)$; temp range 498–573 K (liquid, Antoine eq., Stephenson &
        Malanowski 1987)
    0.253*   (100.26°C, pressure gauge, Sasse et al. 1988)
    $\log (P/mmHg) = 7.17666 - 2243.665/(t/°C + 126.236)$; temp range 100.26–149.23°C (Antoine eq. derived from
        exptl. data, liquid phase, Sasse et al. 1988)
    $\log (P/kPa) = (8.76 \pm 0.50) - (4501 \pm 250)/(T/K)$; temp range 451–497 K (Antoine eq. from exptl. data, transpi-
        ration method, Piacente & Scardala 1990; quoted, Pompili & Piacente 1990)
    $\ln (P/kPa) = 21.25 - 10946/(T/K)$; temp range 501–523 K (transpiration method, Piacente et al. 1991)
    $\ln (P/kPa) = 25.35 - 12399/(T/K)$; temp range 376–438 K (torsion method, Piacente et al. 1991)
    $\ln (P/kPa) = 18.38 - 8349/[(T/K) + 58]$; temp range 343–523 K (transpiration, torsion and Knudsen methods,
        Antoine eq., Piacente et al. 1991)

90.1*   (179.916°C, static-differential pressure, measured range 179.916–314.820°C, Morgan & Kobayashi
        1994)

0.721*, 0.801 (114, 115°C, torsion-effusion, measured range 386–425 K, Piacente et al. 1994)

log (P/kPa) = 13.57 – 6459/(T/K); temp range 388–413 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 14.25 – 6726/(T/K); temp range 387–423 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.92 – 6591/(T/K); temp range 386–425 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.96 – 6608/(T/K); temp range ~ 386–425 K, ΔH_V = 126 kJ mol^{-1} (selected Antoine eq. based
        on exptl. data, torsion-effusion method, Piacente et al. 1994)

3.30×10^{-5} (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)

2.37×10^{-5} (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant (Pa·m³/mol):

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

12.53   (HPLC-k′ correlation, Coates et al. 1985)

12.0; 10.5   (calculated-fragment const; calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Biodegradation: microbial degradation $t_{1/2}$ < 31 d by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.36.1
Reported vapor pressures of tetracosane 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		Zwolinski & Wilhoit 1971		Sasse et al. 1988		Piacente et al. 1990	
summary of literature data		selected values		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						run A	
183.8	133.3	175.9	66.66	100.26	0.255	183.85	85.11
219.6	666.6	188.0	133.3	110.25	0.613	185.85	100.0
237.6	1333	201.1	266.6	120.21	1.560	187.85	97.72
255.3	2666	220.5	666.6	130.15	3.506	189.85	107.2
276.3	5333	236.8	1333	139.93	7.386	193.85	134.9
288.4	7999	391.3	101325	140.09	7.506	195.85	151.4
305.2	13332			149.92	14.80	For run A:-	
330.3	66661	bp/°C	391.3	149.97	14.80	eq. 1	P/kPa
358.0	53329			159.77	28.53	A	8.17
386.4	101325	eq. 2	P/mmHg	159.62	52.13	B	4221
		A	7.0976	179.45	91.06	For temp range: 457–469 K	
mp/°C	51.1	B	2112.0	189.23	148.9	Run B	

TABLE 2.1.1.1.36.1 *(Continued)*

Stull 1947		Zwolinski & Wilhoit 1971		Sasse et al. 1988		Piacente et al. 1990	
summary of literature data		selected values		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		C	109.6			187.85	104.7
				eq. 2	P/mmHg	192.85	138.0
				A	7.16777	197.85	182.0
				B	2243.665	206.85	288.4
				C	126.336	209.85	295.1
						212.35	316.2
						215.85	426.6
						216.85	436.5
						217.35	446.7
						217.88	457.1
						222.35	588.8
						223.35	616.6
						for run B:-	
						eq. 1	P/kPa
						A	9.53
						B	4843
						for temp range: 461–496 K	

2.

Piacente et al. 1990 (cont'd)		Piacente et al. 1991					
transpiration method		transpiration method		torsion method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
run C				cell B		cont'd	
177.85	61.66	227.85	537.0	109.05	0.955	136.85	9.772
184.85	79.43	230.85	602.6	118.35	1.514	138.85	11.22
187.85	85.11	234.85	741.3	122.35	2.089	141.85	13.49
189.85	97.72	238.85	871.0	126.35	2.291	142.85	14.79
192.35	102.3	240.85	933.3	129.35	3.020	144.85	15.85
193.85	117.5	242.85	1096	131.35	3.388	147.85	19.05
194.85	141.25	245.85	1175	134.35	4.365	148.85	21.38
196.85	123.0	246.85	1259	136.35	4.898	149.85	23.44
201.35	141.25	247.85	1047	138.35	6.457	152.35	26.30
205.85	199.5	249.85	1148	141.35	7.943	154.85	29.51
209.85	245.5			143.35	10.23	158.85	39.81
212.85	288.4	For transpiration data:		145.35	11.75	160.35	44.67
213.85	302.0	eq. 1a	P/kPa	147.35	13.80	162.35	51.29
		A	21.25 ± 1.08	cell D		cell D	
		B	10946 ± 554	123.85	2.951	126.85	2.344
for transpiration data:				126.85	3.981	130.85	3.548
eq. 1	P/kPa			129.85	4.677	134.8513885	4.577
A	8.31 ± 1.08			133.85	5.888	139.85	5.888
B	4314 ± 211			135.85	7.079	140.85	6.457
for temp range: 451–487 K				137.85	8.128	142.85	9.333
				139.85	8.128	144.85	10.47
overall vapor pressure eq. by				142.85	9.333	147.85	12.88

(Continued)

TABLE 2.1.1.1.36.1 (*Continued*)

Piacente et al. 1990 (cont'd)		Piacente et al. 1991			
transpiration method		**transpiration method**		**torsion method**			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
weighted slopes and intercepts				145.85	14.125	149.85	15.14
eq. 1	P/kPa			148.85	18.20	152.85	17.78
A	8.76 ± 0.50			151.85	36.31	153.85	18.62
B	4501 ± 250			cell A		156.85	22.39
				102.85	0.7413	162.85	33.11
$\Delta H_V/(kJ\ mol^{-1}) = 86 \pm 5$				104.85	0.8511	164.85	36.31
at 474 K				106.95	0.9772		
				109.85	1.2303	for torsion method data:-	
				114.85	1.5849	eq. 1a	P/kPa
				118.85	2.344	A	25.35 ± 0.60
				126.85	4.169	B	12399 ± 575
				127.85	4.898		
				129.85	5.623		
				131.85	6.918		
				133.85	8.128		

3.

Piacente et al. 1991 (cont'd)		Piacente et al. 1994					
Knudsen effusion		**torsion-effusion**					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		run a		run b		run c	
69.85	0.010	114.85	0.801	113.85	0.721	112.85	0.721
76.85	0.0282	120.85	1.60	117.85	1.12	113.85	0.801
83.85	0.0617	125.85	2.40	120.85	1.44	115.85	0.881
91.85	0.1995	128.85	3.20	123.85	2.08	117.85	1.12
119.35	1.995	132.35	4.33	127.85	2.88	119.85	1.44
		134.85	5.61	130.85	4.17	121.85	1.76
bp/K	664.3	138.35	7.37	133.85	5.29	124.85	2.32
mp/K	323.9	139.85	8.49	136.85	6.89	125.85	2.56
				138.85	8.49	126.85	2.80
eq. for transpiration, torsion		eq. 1	P/kPa	140.85	10.1	128.85	3.12
and Knudsen effusion		A	13.57 ± 0.26	143.85	12.8	130.85	4.17
eq. 3a	P/kPa	B	6459 ± 106	155.85	17.1	131.85	4.65
A	18.38 ± 0.34	temp range: 388–413 K		159.85	21.6	133.85	5.61
B	8349 ± 460					136.85	7.21
C	58 ± 15			eq. 1	P/kPa	139.85	9.29
$\Delta H_{fus}/(kJ\ mol^{-1}) = 58.893$				A	14.25 ± 0.12	142.85	11.9
$\Delta H_{sub}/(kJ\ mol^{-1}) = 162.0$				B	6726 ± 49	144.85	14.1
at 298.15 K				temp range: 387–423 K		146.85	17.0
						151.85	25.3
Morgan & Kobayashi 1994				selected vapor pressure eq.			
differential pressure gauge				eq. 1	P/kPa	eq. 1	P/kPa
t/°C	P/Pa			A	13.96 ± 0.30	A	13.92 ± 0.13
				B	6608 ± 100	B	6591 ± 0.51
179.916	90.1					temp range: 387–423 K	
189.925	154.7			$\Delta H_V/(kJ\ mol^{-1}) = 126 \pm 2$			
199.931	257			at 405 K			

TABLE 2.1.1.1.36.1 *(Continued)*

Piacente et al. 1991 (cont'd)		Piacente et al. 1994					
Knudsen effusion		**torsion-effusion**					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
209.939	415.6						
219.946	652.9			mp/K	322		
229.950	1001			$\Delta H_{fus}/(kJ\ mol^{-1}) = 54.9$			
239.960	1506			$\Delta H_{sub}/(kJ\ mol^{-1}) = 180.9 \pm 2$			
249.971	2209			at 298.15 K			
259.979	3176						
260.979	4489						
284.980	7303						
299.980	11470						
314.820	17460						
data fitted to Wagner eq.							
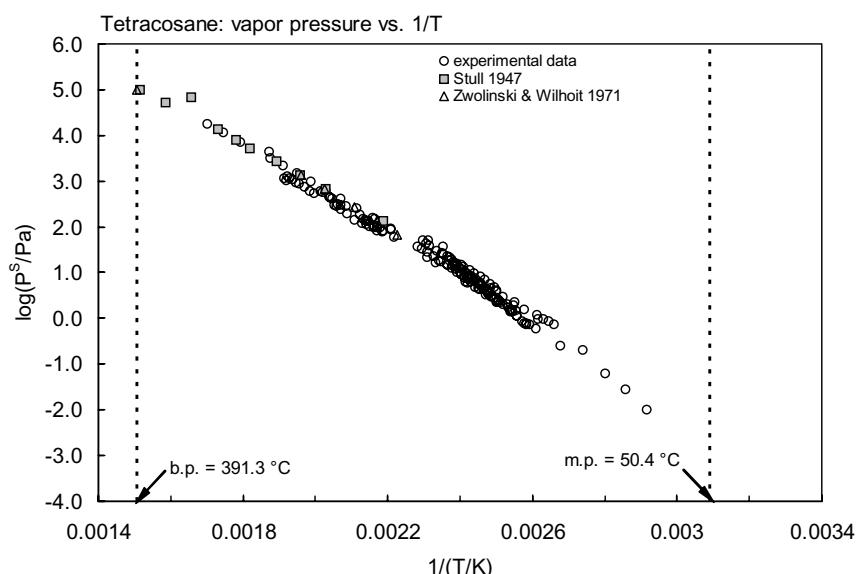
FIGURE 2.1.1.1.36.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tetracosane.

2.1.1.1.37   *n*-Hexacosane
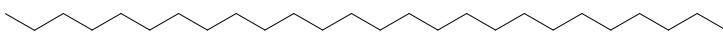
Common Name: Hexacosane
Synonym: cerane
Chemical Name: *n*-hexacosane
CAS Registry No: 631-01-3
Molecular Formula: $C_{26}H_{54}$; $CH_3(CH_2)_{24}CH_3$
Molecular Weight: 366.707
Melting Point (°C):
    56.1   (Lide 2003)
Boiling Point (°C):
    412.2   (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³):
    0.8032, 0.7998   (20°C, 25°C, Dreisbach 1959)
    0.8032   (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
    584.6   (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
    456.6   (20°C, calculated-density)
    457   (Wang et al. 1992)
Enthalpy of vaporization, ΔH_V (kJ/mol):
    64.806   (bp, Dreisbach 1959)
    131.2   (calculated, Chickos & Hanshaw 2004)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    32.3, 59.5; 95.3   (53.35, 56.35°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    289.03, 259.1   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K): F: 0.495 (mp at 56.1°C)

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

    1.7×10^{-3}; 1.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
    1.33×10^{-10} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)

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*   (204.0°C, summary of literature data, temp range 204.0–399.8°C, Stull 1947)
    log (P/mmHg) = 7.57689 – 2692.73/(161.2 + t/°C); temp range 278–500°C (Antoine eq. for liquid state, Dreisbach 1959)
    log (P/mmHg) = 7.1096 – 2164.3/(99.6 + t/°C) (Antoine eq., Kudchadker & Zwolinski 1966)
    66.66*   (192.5°C, derived from compiled data, temp range 192.5–412.2°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.1096 – 2164.3/(99.6 + t/°C); temp range 192.6–412.2°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 21605.7/(T/K)] + 9.899820; temp range 204–399.8°C (Antoine eq., Weast 1972–73)
    log (P_L/kPa) = 6.2345 – 2164.3/(T/K – 173.55); temp range 466–685 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 9.44384 – 4935.969/(T/K); temp range 478–530 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
    log (P/kPa) = (9.93 ± 0.50) – (5168 ± 200)/(T/K); temp range 455–519 K, (Antoine eq. from exptl. data, transpiration, Piacente & Scardala 1990; Pompili & Piacente 1990)
    ln (P/kPa) = 18.63 – 9892/(T/K); temp range 506–546 K (transpiration method, Piacente et al. 1991)
    ln (P/kPa) = 28.91 – 14285/(T/K); temp range 391–442 K (torsion method, Piacente et al. 1991)
    ln (P/kPa) = 17.76 – 8050/[(T/K) + 72]; temp range 356–546 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)
    log (P/kPa) = 14.50 – 7084/(T/K); temp range 420–437 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.75 – 6765/(T/K); temp range 391–433 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.65 – 6748/(T/K); temp range 392–431 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 14.01 – 6682/(T/K); temp range ~ 392–437 K, ΔH_V = 132 kJ mol^{-1} (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)

5.03×10^{-6} (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)

2.82×10^{-6} (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant (Pa·m^3/mol):

    21200   (calculated-P/C, Eastcott et al. 1988)

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

    13.0, 11.4   (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

    Biodegradation: microbial degradation $t_{1/2}$ < 31 d by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.37.1

Reported vapor pressures of hexacosane 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		Zwolinski & Wilhoit 1971		Piacente et al. 1990			
summary of literature data		selected values		transpiration		transpiration (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				run A		run C	
204.0	133.3	192.5	66.66	187.85	64.57	182.35	37.15
240.0	666.6	204.8	133.3	194.35	74.13	188.85	54.95
257.4	1333	218.3	266.6	197.35	91.20	193.35	70.79
275.8	2666	138.0	666.6	197.85	100.0	196.85	89.13
295.2	5333	254.6	527.75	198.35	97.72	199.85	104.7
307.8	7999	412.2	101325	199.85	109.65	202.35	123.0
323.2	13332			202.85	129.8	203.85	131.8
348.4	66661			205.85	131.8	204.85	112.2
374.5	53329	bp/°C	412.2	208.85	162.2	206.85	134.9
399.8	101325			211.85	251.2	210.85	229.1
		eq. 2	P/mmHg	214.85	263.0	215.35	288.4
mp/°C	56.6	A	7.1096	eq. for run A:-		218.85	263.0
		B	2164.3	eq. 1	P/kPa	221.85	309.0
		C	99.6	A	10.40 ± 0.42	223.35	346.7

(Continued)

TABLE 2.1.1.1.37.1 (*Continued*)

Stull 1947		Zwolinski & Wilhoit 1971		Piacente et al. 1990			
summary of literature data		selected values		transpiration		transpiration (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				B	5355 ± 198	243.35	691.8
				for temp range: 461–488 K		245.85	812.8
				run B		eq. for run C:-	
				202.35	100	eq. 1	P/kPa
				209.35	128.8	A	9.53 ± 0.21
				215.85	166.0	B	4979 ± 103
				220.85	269.2	temp range: 455.5–519 K	
				224.85	295.1		
				227.35	331.1	overall vapor pressure eq. by	
				229.35	407.4	weighted slopes and intercepts	
				234.85	457.1	eq. 1	P/kPa
						A	9.93 ± 0.50
				eq. 1	P/kPa	B	5168 ± 200
				A	10.09 ± 0.64		
				B	5289 ± 315	$\Delta H_V/(kJ\ mol^{-1}) =$	
				for temp range: 475.5–508 K		at 488 K	99 ± 4

2.

Piacente et al. 1991							
transpiration method		torsion method		torsion (continued)		torsion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		cell E		cell A		cell B	
232.85	354.8	131.35	1.202	141.35	1.479	138.85	3.020
238.35	616.6	132.35	1.380	143.35	1.950	142.85	4.571
242.85	616.6	134.35	1.585	145.35	2.692	144.85	4.169
242.85	616.6	136.35	1.778	146.35	3.162	144.85	4.898
246.35	575.4	137.35	1.995	146.85	3.715	147.35	6.166
247.85	660.7	139.35	2.570	147.35	4.169	150.35	6.457
249.35	758.6	140.85	3.020	147.85	4.898	153.85	9.550
251.35	871.0	142.35	3.388	148.35	5.623	154.35	9.120
252.35	933.3	146.35	5.129	148.85	6.310	154.35	9.550
254.35	933.3	148.35	6.166	149.35	7.586	154.85	9.550
255.85	1023	150.35	6.918	150.35	9.120	155.85	10.72
256.35	871.0	153.35	7.762	152.35	10.47	155.85	10.96
258.85	1047	155.35	9.120	154.35	11.22	158.85	13.80
259.35	1148	158.35	12.30	165.35	12.88	cell A	
261.85	1288	160.35	14.13	158.35	15.49	132.85	2.455
262.85	1288	163.35	17.38	160.35	18.62	135.35	2.951
266.35	1230	165.35	20.42	cell A		138.85	3.890
266.35	1259	167.35	23.99	117.85	0.490	142.35	5.129
268.35	1445	169.35	28.18	123.85	0.741	143.85	5.623
269.35	1413			126.85	0.977	145.35	6.310
271.85	1380			128.35	0.977	146.85	7.586
272.85	1585			129.35	1.230	147.35	7.413
272.85	1514			131.35	1.479	147.85	8.511
				133.35	1.698	148.85	9.550
eq. 1a	P/kPa			134.35	1.950	150.35	9.120

TABLE 2.1.1.1.37.1 (*Continued*)

Piacente et al. 1991

transpiration method		torsion method		torsion (continued)		torsion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
A	18.63 ± 1.03			135.35	2.188	150.85	10.00
B	9892 ± 552			136.35	2.455	151.85	10.47
				137.35	2.951	152.35	12.88
				138.35	3.467	152.85	13.18
				139.35	3.890	153.85	14.13
				141.35	4.677	155.85	15.85
				143.35	5.379		
						eq. 1a	P/kPa
						A	28.91 ± 0.40
						B	14285 ± 345

3.

Piacente et al. 1991 (cont'd) / **Piacente et al. 1994**

Knudsen effusion		torsion-effusion		torsion-effusion (continued)		torsion-effusion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		run a		run b		run c	
83	0.01995	146.85	4.01	117.85	0.320	118.85	0.320
92	0.04677	147.85	4.49	120.85	0.401	124.85	0.481
102	0.1514	148.85	5.13	124.85	0.481	127.85	0.641
111	0.2818	149.85	5.77	128.85	0.801	130.85	0.801
119	0.5623	150.85	6.42	131.85	1.120	133.85	1.12
		151.85	7.05	134.85	1.52	136.85	1.60
bp/K	658.2	152.85	7.69	137.85	2.08	139.85	2.08
mp/K	329.4	153.85	8.33	141.85	2.88	142.85	2.72
		154.85	9.13	145.85	4.17	146.85	3.85
eq. for transpiration, torsion		155.85	9.61	149.85	5.77	151.85	6.09
and Knudsen effusion		156.85	10.9	156.85	10.7	154.85	7.85
eq. 3a	P/kPa	157.85	11.7	159.85	13.5	157.85	10.4
A	17.76 ± 0.46	159.85	13.3				
B	8050 ± 460	161.85	15.5				
C	72 ± 10	163.85	18.9				
				eq. 1	P/kPa	eq. 1	P/kPa
		eq. 1	P/kPa	A	13.75 ± 0.29	A	13.65 ± 0.29
		A	14.50 ± 0.36	B	6765 ± 119	B	6748 ± 120
ΔH_{fus}/(kJ mol^{-1}) = 60.70		B	7084 ± 153	temp range: 391–433 K		temp range: 392–431 K	
		temp range: 420–437 K					
ΔH_{sub}/(kJ mol^{-1}) = 177.2		overall vapor pressure eq.					
at 298.15 K				eq. 1	P/kPa		
				A	14.01 ± 0.30		
				B	6882 ± 50		
				ΔH_V/(kJ mol^{-1}) =			
				at 414 K	132 ± 1		
				mp/K	329		
				ΔH_{fus}/(kJ mol^{-1}) = 59.9			
				ΔH_{sub}/(kJ mol^{-1}) = 191.5 ± 1			
				at 298.15 K			
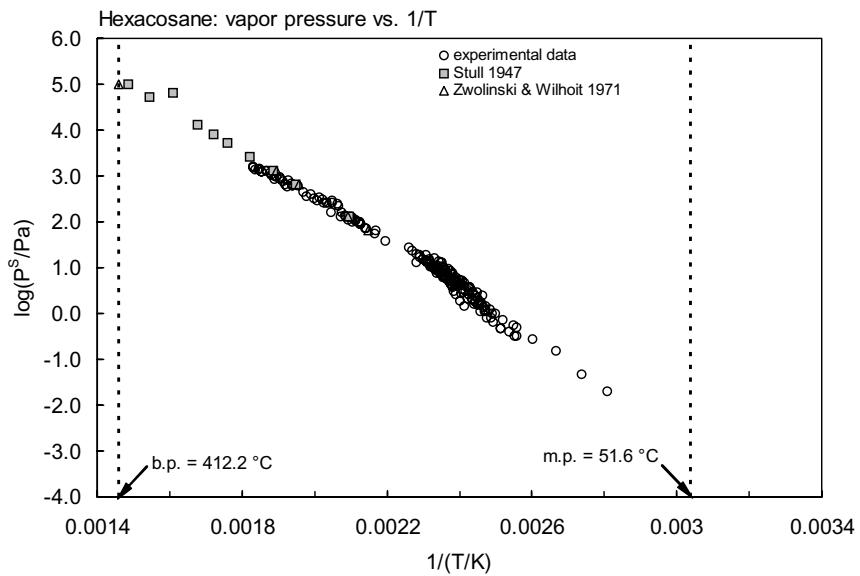
FIGURE 2.1.1.1.37.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexacosane.

2.1.1.2   Cycloalkanes

2.1.1.2.1   Cyclopentane

Common Name: Cyclopentane
Synonym: pentamethylene
Chemical Name: cyclopentane
CAS Registry No: 287-92-37
Molecular Formula: C_5H_{10}
Molecular Weight: 70.133
Melting Point (°C):
    –93.4   (Lide 2003)
Boiling Point (°C):
    49.3   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.7457   (Weast 1984)
    0.7454, 0.7440   (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    94.10   (20°C, calculated-density; McAuliffe 1966)
    99.5   (calculated-Le Bas method at normal boiling point, Abernethy et al. 1988; Mackay & Shiu 1990)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    28.527, 27.296 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    0.609   (Riddick et al. 1986)
    4.9, 0.34, 0.60; 5.84 (–151.15, –135.15, –93.45°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    45.96, 40.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end
    of this section.):
    156   (shake flask-GC, McAuliffe 1963, 1966)
    342*   (shake flask-GC, measured range 5.11–45.21°C, Pierotti & Liabastre 1972)
    160*   (shake flask-GC, measured range 25–153.1°C, Price 1976)
    160   (shake flask-GC, Krzyzanowska & Szeliga 1978)
    164   (shake flask-GC, Groves 1988)
    156*   (IUPAC "tentative" best, IUPAC Solubility Data Series, Shaw 1989)
    166*   (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–426.3 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    27250*   (14.25°C, static method-manometry, measured range –47.24 to 14.25°C, Ashton et al. 1943)
    34890*   (20.2°C, ebulliometry-manometer, measured range 15.7–50°C, Willingham et al. 1945)
    log (P/mmHg) = 6.87798 – 1119.208/(230.738 + t/°C); temp range 15.7–50.0°C (Antoine eq. from exptl. data,
        ebulliometry-manometer, Willingham et al. 1945)
    43150*   (Antoine eq. regression, temp range –68 to 49.4°C, Stull 1947)
    42330   (calculated from exptl. determined data, Dreisbach 1955; quoted, Hine & Mookerjee 1975)
    log (P/mmHg) = 6,88676 – 1124.162/(231.361 + t/°C); temp range –25 to 110°C (Antoine eq. for liquid state,
        Dreisbach 1955)
    29036*   (selected exptl. data, temp range –39 to 230°C, Pasek & Thodos 1962)

42400   (interpolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)

42330*   (derived from compiled data, temp range –40.4 to 71.6°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.88676 – 1124.162/(231.361 + t/°C); temp range –40.4 to 71.6°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 7411.1/(T/K)] + 7.940722; temp range –68 to 49.3°C (Antoine eq., Weast 1972–73)

log (P/atm) = [1– 322.386/(T/K)] × 10^{0.818603 – 7.52365 × 10^{-4}·(T/K) + 8.27395 × 10^{-7}·(T/K)^2}; temp range: 190.20–503.20 K (Cox eq., Chao et al. 1983)

42570, 42320   (calculated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.25832 – 1240.438/(242.957 + t/°C); temp range –47.25 to 14°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.82877 – 1133.199/(232.415 + t/°C), temp range 15.7–50.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

42320   (interpolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.88676 – 1124.162/(231.36 + t/°C); temp range –40 to 72°C (Antoine eq., Dean 1985, 1992)

42400   (selected lit., Riddick et al. 1986)

log (P/kPa) = 6.04584 – 1142.30/(233.463 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

42340   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.0080 – 1122.21/(–42.011 + T/K); temp range 280–311 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.08918 – 1174.132/(–34.864 + T/K); temp range 322–384 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.41769 – 1415.096/(–0.66 + T/K) temp range 381–455 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.77782 – 1749.65/(48.533 + T/K); temp range 452–511 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 29.1547 – 2.3512 × 10^3/(T/K) – 7.6965·log (T/K) – 1.6212 × 10^{-10}·(T/K) + 3.125 × 10^{-6}·(T/K)^2; temp range 179–512 K (vapor pressure eq., Yaws 1994)

35000*   (20.14°C, differential pressure gauge, measured range –68.59 to 70.06°C, Mokbel et al. 1995)

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.):

18800   (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

13310; 18380   (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

18500; 19100, 18600   (recommended; calculated-P/C, Mackay & Shiu 1981)

17550   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

19030   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

16617*   (27.9°C, EPICS-GC, measured range 27.9–45°C, Hansen et al. 1993)

ln [H/(kPa·m^3/mol)] = –3351/(T/K) + 14.0; temp range 27.9–45°C (EPICS-GC, Hansen et al. 1993)

12796   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 5.162 – 1302/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

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

3.00   (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)

3.00   (recommended, Sangster 1989, 1993)

3.00   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

     Volatilization:
     Photolysis:

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

$k_{O(3P)} = 1.30 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) (Herron & Huie 1973)

$k_{OH} = (4.72 \pm 0.28) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH} (calc) = 5.80×10^{-12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

$k_{OH} = 5.40 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1979)

$k_{OH} = 5.40 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}; $k_{O(3P)} = 1.3 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atoms at room temp. (Gaffney & Levine 1979)

$k_{OH} = 6.20 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K and 5.18×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K and 5.24×10^{-12} cm^3·molecule^{-1} s^{-1} at 299 K and 4.43×10^{-12} cm^3·molecule^{-1} s^{-1} at 300 K (Atkinson 1985)

$k_{OH} = (3.12 \pm 0.23) \times 10^{12}$ cm^3 mol^{-1} s^{-1} at 298 $\pm$ 2 K (flash photolysis-resonance absorption technique, Jolly et al. 1985)

$k_{OH} = 5.02 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 295 K, measured range 295–491 K (Droege & Tully 1987)

$k_{OH}* = 5.16 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = 5.16 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K with an estimated lifetime of 27 h in summer daylight (Altshuller 1991)

$k_{OH}* = 5.02 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

$k_{OH}* = 4.83 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant k = 5.16×10^{-12} cm^3 molecule^{-1} s^{-1} with hydroxyl radical in air at 298 K (Atkinson 1990; Altshuller 1991) with an estimated lifetime of 27 h, based on reaction rate with OH radical in summer daylight (Altshuller 1991).

TABLE 2.1.1.2.1.1
Reported aqueous solubilities of cyclopentane at various temperatures

Pierotti & Liabastre 1972		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC/FID		shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
5.11	338.6	25.0	160	5	339	25	168
15.21	341.7	40.1	163	15	342	40.1	175
25.11	341.9	55.7	180	25	156	55.7	195
35.21	368.5	99.1	296	30	160	99.1	343
45.21	341.5	118.0	372	40	350	118	468
		137.3	611	60	500	137.3	701
		153.1	792	80	750	153.1	974
ΔH_{sol}/(kJ mol^{-1}) = –2.50				100	1100		
25°C				120	1600		
		ΔH_{sol}/(kJ mol^{-1}) = –2.80		140	2600		
		25°C		160	3850		
				180	6700		
				200	14000		
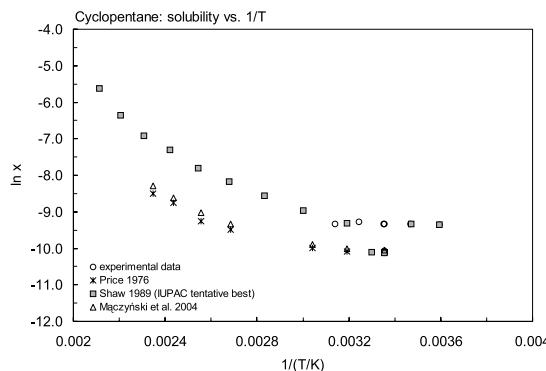
FIGURE 2.1.1.2.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for cyclopentane.

TABLE 2.1.1.2.1.2
Reported vapor pressures of cyclopentane 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)		
log P = A + B/(T/K) + C·log (T/K) + D[P/(T/K)²]			(5)
log P = A – B/T(T/K) – C·log (T/K) + D × 10⁻³(T/K) – E × 10⁻⁸(T/K)²			(6)

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$
$$\log P = A - B/(C + t/°C) \quad (2) \qquad \ln P = A - B/(C + t/°C) \quad (2a)$$
$$\log P = A - B/(C + T/K) \quad (3)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$
$$\log P = A + B/(T/K) + C \cdot \log (T/K) + D[P/(T/K)^2] \quad (5)$$
$$\log P = A - B/T(T/K) - C \cdot \log (T/K) + D \times 10^{-3}(T/K) - E \times 10^{-8}(T/K)^2 \quad (6)$$

1.

Ashton et al. 1943		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
static method-manometry		ebulliometry		summary of literature data		selected experimental data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–47.24	830.6	15.707	28956	–68.0	133.3	–39.064	1571
–38.35	1570	20.196	34892	–49.6	666.6	9.335	21949
–31.63	2446	25.598	43322	–40.4	1333	15.722	29036
–24.7	3753	31.172	53656	–30.1	2666	48.146	97608
–18.6	5360	37.119	66760	–18.6	5333	57.885	133322
–12.91	7350	43.574	83722	–11.3	7999	71.612	1999836
–7.29	9875	48.131	97608	–1.30	13332	100.005	4197790
–1.93	12931	48.621	99205	13.8	26664	230.065	4023402
4.47	17569	49.073	100698	31.0	53329		
9.33	21949	49.587	102401	49.3	101325	bp/°C	49.307
14.25	27250	50.031	103921				
				mp/°C	–93.7	Frost-Kalkwarf equation:	
bp/°C	49.20					derived from exptl. data	
mp/°C	–93.62	bp/°C	49.262			eq 5	P/mmHg
						A	21.62180
eq. 6	P/mmHg	eq. 2	P/mmHg			B	–2131.85
A	30.957385	A	6.87798			C	–4.83947
B	2298.386	B	1119.208			D	1.41701
C	8.91170	C	230.738				
D	4.385677					Frost-Kalkwarf equation:	
E	1.054940					calculated from molecular	
						structures, normal bp and	

TABLE 2.1.1.2.1.2 (*Continued*)

Ashton et al. 1943		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
static method-manometry		ebulliometry		summary of literature data		selected experimental data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ΔH_V/(kJ mol^{-1}) = 29.21						deviations of resulting v.p.:-	
at 25°C						eq 5	P/mmHg
						A	21.63300
						B	−2132.5
						C	−4.84313
						D	1.41701

2.

Zwolinski & Wilhoit 1971		Mokbel et al. 1995	
selected values		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa
−40.4	1333	−68.59	138
−30.1	2666	−59.24	313
−23.6	4000	−49.42	692
−18.6	5333	−39.51	1446
−14.7	6666	−39.42	1456
−11.3	7999	−29.66	2775
−5.80	10666	−29.53	2781
−1.30	13332	−19.77	5034
7.28	19998	−19.64	5057
13.78	26664	−9.86	8679
19.08	33331	−9.73	8718
23.57	39997	0.15	14340
31.01	53329	0.22	14430
37.08	66661	10.11	22750
42.35	79993	10.17	22840
46.78	93326	20.08	34860
47.627	95992	20.14	35000
48.453	98659	30.27	51930
49.262	101325	40.23	74670
		50.14	104580
		60.12	143100
eq. 2	P/mmHg	65.10	166090
A	6.88676	70.06	191640
B	1124.162		
C	231.361	Wagner eq. given in ref.	
bp/°C	49.262		
ΔH_V/(kJ mol^{-1}) =			
at 25°C	28.53		
at bp	27.30		
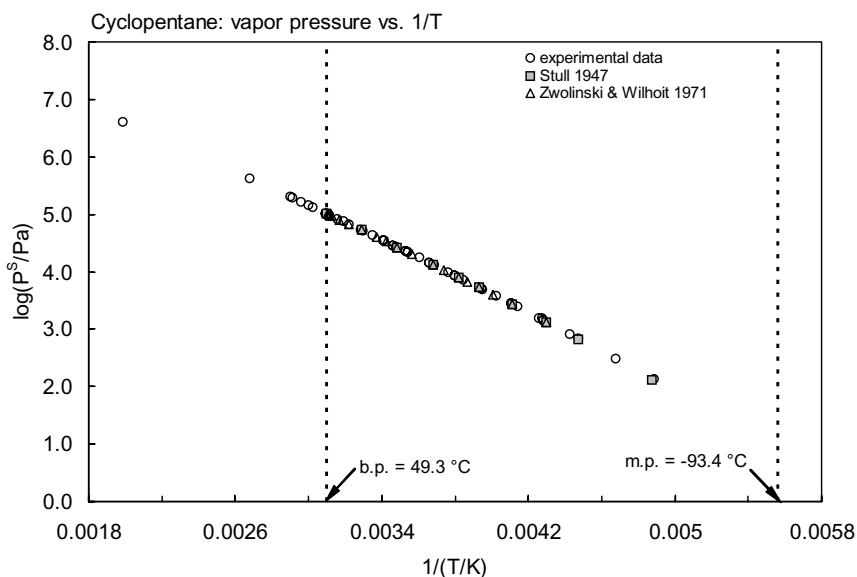
FIGURE 2.1.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for cyclopentane.

TABLE 2.1.1.2.1.3
Reported Henry's law constants of cyclopentane at various temperatures

	Hansen et al. 1993
	EPICS-GC
t/°C	H/(kPa m³/mol)
27.9	16.617
35.8	24.318
45.0	30.398

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

	H/(kPa m³/mol)
A	14 ± 2.03
B	3351 ± 633
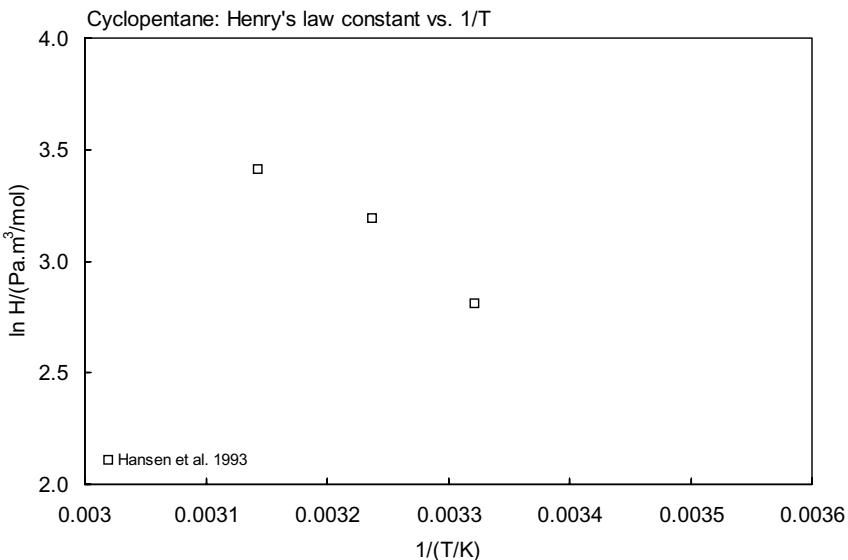
FIGURE 2.1.1.2.1.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclopentane.

2.1.1.2.2   Methylcyclopentane

Common Name: Methylcyclopentane
Synonym:
Chemical Name: methylcyclopentane
CAS Registry No: 96-37-3
Molecular Formula: C_6H_{12}
Molecular Weight: 84.159
Melting Point (°C):
    –142.42   (Lide 2003)
Boiling Point (°C):
    71.8   (Lide 2003)
Density (g/cm³ at 25°C):
    0.7487, 0.7439   (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm³/mol):
    112.4, 113.1   (20°C, 25°C, calculated from density)
    121.7   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.59, 29.08   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.929   (Riddick et al. 1986)
    6.93   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    53.01, 43.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    42.6   (shake flask-GC, McAuliffe 1963)
    42.0   (shake flask-GC, McAuliffe 1966)
    41.8   (shake flask-GC, Price 1976)
    45.0   (partition coefficient-GC, Rudakov & Lutsyk 1979)
    43.0   (recommended, IUPAC Solubility Data Series, Shaw 1989)
    74.8   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    16680   (22.75°C, ebulliometry-manometer, measured range 15.0–22.6°C, Willingham et al. 1945)
    log (P/mmHg) = 6.86283 – 1186.059/(229.042 + t/°C); temp range 15.0–22.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
    17870   (Antoine eq. regression, temp range –53.7 to 71.8°C, Stull 1947)
    18330   (calculated from exptl. determined data, Dreisbach 1955)
    log (P/mmHg) = 6.86283 – 1186.059/(226.042 + t/°C); temp range –5 to 125°C (Antoine eq. for liquid state, Dreisbach 1955)
    18302   (interpolated-Antoine eq., temp range –23.7 to 95.7°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.86283 – 1186.059/(226.042 + t/°C); temp range –23.7 to 95.7°C (Antoine eq., Zwolinski & Wilhoit 1971)
    17850   (interpolated-Antoine eq., temp range –53.7 to 71.8°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 7490.0/(T/K)] + 7.945471; temp range –53.7 to 71.8°C (Antoine eq., Weast 1972–73)
    log (P/atm) = [1– 344.830/(T/K)] × 10^{0.872156 – 9.88091 × 10^{–4}·(T/K) + 10.8367 × 10^{–7}·(T/K)²}; temp range: 183.15–513.15 K (Cox eq., Chao et al. 1983)

18330   (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.99178 – 1188.32/(226.307 + t/°C); temp range 15.035–72.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

18330   (interpolated-Antoine eq., Dean 1985)

log (P/mmHg) = 6.86283 – 1186.059/(226.04 + t/°C); temp range –24 to 96°C (Antoine eq., Dean 1985, 1992)

18400   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.98773 – 1186.059/(226.042 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

18340   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.98551 – 1184.874/(–47.232 + T/K); temp range 288–346 K (Antoine eq., Stephenson & Malanowski 1987)

18400, 17066   (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

log (P/mmHg) = 32.4766 – 2.6434 × 10^3/(T/K) – 8.733·log (T/K) + 2.0749 × 10^{-11}·(T/K) + 3.2158 × 10^{-6}·(T/K)^2; temp range 131–533 K (vapor pressure eq., Yaws 1994)

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

36664   (calculated as $1/K_{AW}$, C_W/C_A reported as exptl., Hine & Mookerjee 1975)

22090, 27810   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

36700; 36700, 36800 (recommended, calculated-P/C, Mackay & Shiu 1981)

25370   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

36934   (calculated-P/C, Eastcott et al. 1988)

36180   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

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

3.37   (recommended, Sangster 1989)

3.37   (Hansch et al. 1995)

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


Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, 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} = 7.10 × 10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson 1990, 1991)

k_{OH} = 7.10 × 10^{-12} cm^3 molecule^{-1} s^{-1} with a estimated lifetime τ = 20 h in summer daylight (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

rate constant k = 7.10 × 10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with hydroxyl radical in air (Atkinson 1990, 1991, Altshuller 1991); and an estimated reaction lifetime τ = 20 h in summer daylight (Altshuller 1991).

2.1.1.2.3   1,1,3-Trimethylcyclopentane
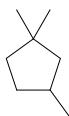
Common Name: 1,1,3-Trimethylcyclopentane
Synonym:
Chemical Name: 1,1,3-trimethylcyclopentane
CAS Registry No: 4516-69-2
Molecular Formula: C_8H_{16}
Molecular Weight: 112.213
Melting Point (°C):
    –142.4   (Lide 2003)
Boiling Point (°C):
    104.9   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7483, 0.7430 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
    146.0   (20°C, calculated-density, Wang et al. 1992)
    166.1   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    36.23, 32.35 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    3.73   (shake flask-GC, Price 1976)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    log (P/mmHg) = 6.80948 – 1275.998/(219.899 + t/°C); temp range 28.9–105.8°C (Antoine eq., ebulliometry-
        manometer measurements, Forziati et al. 1949)
    5300   (calculated from determined data, Dreisbach 1955)
    log (P/mmHg) = 6.80947 – 1275.988/(219.899 + t/°C); temp range 20–140°C (interpolated-Antoine eq. for liquid
        state, Dreisbach 1955)
    5300   (interpolated-Antoine eq., temp range –0.30 to 131.3°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.80947 – 1275.998/(219.899 + t/°C); temp range –0.30 to 131.3°C (interpolated-Antoine eq.,
        Zwolinski & Wilhoit 1971)
    log (P/atm) = [1– 378.056/(T/K)] × 10^{0.848231 – 8.28174 × 10⁻⁴·(T/K) + 8.81168 × 10⁻⁷·(T/K)²}; temp range:
        272.85–404.45 K (interpolated-Cox eq., Chao et al. 1983)
    5300   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.93423 – 1275.928/(219.893 + t/°C); temp range 28.944–105.8°C (extrapolated-Antoine eq. from
        reported exptl. data, Boublik et al. 1984)
    5070   (extrapolated-Antoine eq., temp range 29–106°C, Dean 1985. 1992)
    log (P/mmHg) = 6.80931 – 1275.92/(219.89 + t/°C); temp range 29–106°C (extrapolated-Antoine eq., Dean
        1985, 1992)
    log (P_L/kPa) = 5.93036 – 1273.902/(–53.454 + T/K); temp range 301–379 K (extrapolated-Antoine eq., Stephenson
        & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):
    159000   (calculated-P/C, Mackay & Shiu 1981)

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

    3.28   (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

    3.34   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

    Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976).

2.1.1.2.4 n-*Propylcyclopentane*
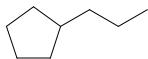
Common Name: *n*-Propylcyclopentane
Synonym:
Chemical Name: *n*-propylcyclopentane
CAS Registry No: 2040-96-2
Molecular Formula: C_8H_{16}
Molecular Weight: 112.213
Melting Point (°C):
    –117.3   (Dreisbach 1955; Lide 2003)
Boiling Point (°C):
    130.937   (Willingham et al. 1945)
    131   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.7763, 07723(20°C, 25°C, Dreisbach 1955)
Molar Volume (cm^3/mol):
    144.6   (20°C, calculated-density)
    166.1   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.197, 34.746(25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    10.04   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    64.45, 57.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    2.04   (shake flask-GC, Price 1976)
    1.77   (shake flask-GC, Krzyzanowska & Szeliga 1978)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    log (P/mmHg) = 6.89887 – 1380.391/(212.610 + t/°C); temp range 51.7–131.9°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
    log (P/mmHg) = 6.30392 – 1384.386/(213.159 + t/°C); temp range 51.9–131.9°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
    1650   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 6.90392 – 1384.386/(213.159 + t/°C); temp range 40–170°C (extrapolated-Antoine eq. for liquid state, Dreisbach 1955)
    1640   (interpolated-Antoine eq., temp range –21.3 to158.2°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.30392 – 1384.386/(213.159 + t/°C); temp range –21.3 to 158.2°C (Antoine eq., Zwolinski & Wilhoit 1971)
    1646   (extrapolated-Antoine eq., Boublik et al. 1973)
    log (P/mmHg) = 6.91061 – 1388.511/(213.615 + t/°C); temp range 51.88–131.97°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1973)
    1640, 5320 (quoted, calculated-bp, Mackay et al. 1982)
    log (P/atm) = [1– 427.713/(T/K)] × 10^{0.865420 – 7.04026 × 10^{-4}·(T/K) + 5.98562 × 10^{-7}·(T/K)^2}; temp range: 313.35–458.95 K (Cox eq., Chao et al. 1983)
    1644   (extrapolated-Antoine eq., temp range 40–186°C, Dean 1985, 1992)
    log (P/mmHg) = 6.88646 – 1460.80/(207.94 + t/°C); temp range 40–186°C (Antoine eq., Dean 1985, 1992)
    log (P$_L$/kPa) = 6.04236 – 1393.284/(–58.949 + T/K); temp range 323–406 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 33.922 – 3.2097 × 10^3/(T/K) – 8.9914·log (T/K) – 3.2992 × 10^{-11}·(T/K) + 2.0684 × 10^{-6}·(T/K)^2; temp range 156–603 K (vapor pressure eq., Yaws 1994)

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

  90200   (calculated-P/C, Mackay & Shiu 1981)
  90430   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

  3.95   (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
  2.65   (calculated-molar volume V_M, Wang et al. 1992)
  4.37   (calculated-fragment const., Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

2.1.1.2.5   Pentylcyclopentane
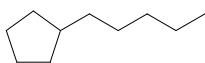
Common Name: Pentylcyclopentane
Synonym: 1-cyclopentylpentane
Chemical Name: pentylcyclopentane
CAS Registry No: 3741-00-2
Molecular Formula: $C_{10}H_{20}$
Molecular Weight: 140.266
Melting Point (°C):
    –83   (Dreisbach 1955; Lide 2003)
Boiling Point (°C):
    180   (Dreisbach 1955; Lide 2003)
Density (g/cm^3 at 20°C):
    0.7912, 0.7874   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
    177.3, 178.1 (20°C, 25°C, calculated-density)
    210.5   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    51.12, 39.94 (25°, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    0.115   (shake flask-GC, Price 1976)
    0.13   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    159   (calculated by formula, Dreisbach 1959)
    log (P/mmHg) = 6.929 – 1526.0/(197.0 + t/°C); temp range 85–220°C (Antoine eq. for liquid state, Dreisbach
        1955)
    152   (extrapolated-Antoine eq., temp range 60–210°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.9414 – 1540.6/(198.8 + t/°C); temp range 60–210°C (Antoine eq., Zwolinski & Wilhoit 1971)

Henry's Law Constant (Pa m^3/mol at 25°C):
    18500   (calculated-P/C, Mackay & Shiu 1981)
    18600   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

2.1.1.2.6   Cyclohexane

Common Name: Cyclohexane
Synonym: hexahydrobenzene, hexamethylene
Chemical Name: cyclohexane
CAS Registry No: 110-82-7
Molecular Formula: C_6H_{12}
Molecular Weight: 84.159
Melting Point (°C):
    6.59   (Lide 2003)
Boiling Point (°C):
    80.73   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7786, 0.7739   (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm³/mol):
    108.1   (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981)
    118.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    32.89, 30.05   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    2.677   (Riddick et al. 1986)
    5.84, 2.68; 9.41   (–87.05, 6.65°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    45.77, 44.55   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C, additional data at other temperatures designated * are compiled at the end of this section.):
    80.0   (shake flask-gravitational method, McBain & Lissant 1951)
    55.0   (shake flask-GC, McAuliffe 1963, 1966)
    88.84*   (shake flask-GC/FID, measured range 5.11–45.21°C, Pierotti & Liabastre 1972)
    56.7   (shake flask-GC/FID, Leinonen & Mackay 1973)
    57.5   (shake flask-vapor extraction-GC/FID, Mackay & Shiu 1975)
    55.8, 50.2, 61.7 (shake flask-GC, Mackay et al. 1975)
    66.5   (shake flask-GC/FID, Price 1976)
    66.5   (shake flask-GC, Krzyzanowski & Szeliga 1978)
    52.0   (23.5°C, elution chromatography, Schwarz 1980)
    72.4   (calculated-HPLC-k′ correlation, converted from reported γ_W, Hafkenscheid & Tomlinson 1983)
    72.8*   (40°C, shake flask-GC, measured range 40–209.06°C, Tsonopoulos & Wilson 1983)
    58.4   (shake flask-GC, Groves 1988)
    58.0*   (IUPAC recommended best value, Shaw 1989a)
    ln x = –301.366 + 12924.45/(T/K) + 43.2980·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)
    ln x = –219.863 + 6693.78/(T/K) + 31.3744·ln (T/K); temp range 290–400 K (eq. derived from direct fit of solubility data, Tsonopoulos 2001)
    60.78   (calculated-liquid-liquid equilibrium LLE data, temp range 278.2–482.2 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    12972   (gas saturation/air-bubbling method, Washburn & Handorf 1935)
    16212*   (30°C, vapor-liquid equilibrium VLE data, measured range 30–80°C, Scatchard et al. 1939)

log (P/mmHg) = 6.65859 – 1040.641/(T/K) – 104.865/(T/K)^2; temp range 30–60°C (VLE data, Scatchard et al. 1939)

10910*   (20.97°C, manometry, measured range 6.33–20.97 °C, Aston et al. 1943b)

11700*   (20.96°C, ebulliometry-manometer, measured range 19.9–81.6°C, Willingham et al. 1945)

log (P/mmHg) = 6.84498 – 1203.526/(222.863 + t/°C); temp range 19.9–81.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

12280*   (calculated-Antoine eq. regression, temp range –45.3 to 80.7°C, Stull 1947)

10253*; 10375 (20.015°C, selected exptl., calculated-Frost-Kalkwarf vapor pressure eq., temp range 293.185–551.225 K, Pasek & Thodos 1962)

log (P/mmHg) = 23.14002 – 2411.8/(T/K) – 5.17900·log (T/K) + 1.84394·[(P/mmHg)/(T/K)^2]; temp range 293.185–551.225 K (Frost-Kalkwarf eq., Pasek & Thodos 1962)

13040*   (static method, measured range 25–75°C, Cruickshank & Cutler 1967)

log (P/mmHg) = 6.85875 – 1212.014/(233.956 + t/°C); temp range 25–75°C (static method, Cruickshank & Cutler 1967)

13010   (calculated from determined data, Dreisbach 1955)

log (P/mmHg) = 6.84498 – 1203.526/(222.863 + t/°C); temp range –20 to 142°C (Antoine eq. for liquid state, Dreisbach 1955)

13159*   (25.26°C, temp range 17.55–80.22°C, Boublik 1960; quoted, Boublik et al. 1984)

13014*   (interpolated-Antoine eq., temp range 6.59–105.2°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.84130 – 1201.531/(222.647 + t/°C); temp range 6.59–105.2°C (Antoine eq., Zwolinski & Wilhoit 1971)

11170   (interpolated-Antoine eq., temp range –45.3 to 257.5°C, Weast 1972–73)

log (P/mmHg) = [–0.2185 × 7830.9/(T/K)] + 7.662126; temp range –45.3 to 257.5°C (Antoine eq., Weast 1972–73)

log (P/atm) = [1– 353.663/(T/K)] × 10^{0.881199 – 9.58655 × 10^{-4}·(T/K) + 9.72305 × 10^{-7}·(T/K)^2}; temp range 227.85–553.64 K (Cox eq., Chao et al. 1983)

13010, 13040 (interpolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 5.97561 – 1206.731/(223.223 + t/°C), temp range 19.9–81.6°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 6.98226 – 1211.248/(223.869 + t/°C); temp range 25–75°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.00569 – 1223.273/(225.089 + t/°C); temp range 17.55–80.22°C (Antoine eq. from reported exptl. data of Cruickshank & Cutler 1967, Boublik et al. 1984)

13020   (interpolated-Antoine eq., temp range 20–81°C, Dean 1985, 1992)

log (P/mmHg) = 6.84130 – 1201.53/(222.65 + t/°C); temp range 20–81°C (Antoine eq., Dean 1985, 1992)

13040   (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.96407 – 1200.31/(222.504 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

13070   (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_S$/kPa) = 7.2778 – 1747.2/(26.84 + T/K); temp range 223–280 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.9682 – 1201.531/(–50.503 + T/K); temp range 293–335 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.03245 – 1244.124/(–44.911 + T/K); temp range 353–414 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.36849 – 1519.732/(–4.032 + T/K); temp range 412–491 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 7.37347 – 2683.075/(159.31 + T/K); temp range 489–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)

12920, 1730 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

log (P/mmHg) = 48.5529 – 3.0874 × 10^3/(T/K) –15.521·log (T/K) + 7.383 × 10^{-3}·(T/K) + 6.3563 × 10^{-12}·(T/K)^2; temp range 280–554 K (vapor pressure eq., Yaws 1994)

12068*   (23.363°C, comparative ebulliometry, measured range 281–552 K, data fitted to Wagner eq., Ewing & Ochoa 2000)

16230, 36180   (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

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.):

   19860   (calculated-P/C, Mackay & Shiu 1975)
   19690   (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
   18380, 27810 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
   18000   (recommended; Mackay & Shiu 1981)
   22092   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
   5532, 17935, 19353, 1450 (bubble column non-equilibrium measurement, EPICS-GC, direct concentration. ratio, calculated-UNIFAC activity coeff., Ashworth et al. 1988)
   17935*   (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
   ln [H/(atm·m^3/mol)] = 9.141 – 3238/(T/K); temp range: 10–30°C (EPICS measurements, Ashworth et al. 1988)
   19980   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
   37190*   (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
   ln ($1/K_{AW}$) = –12.90 + 3228/(T/K); temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
   15062   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
   log K_{AW} = 5.154 – 1279/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

   2.46   (calculated-π substituent constant, Hansch et al. 1968)
   3.44   (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)
   3.40   (Cramer 1977)
   3.18, 3.48, 3.48   (calculated-fragment const., Rekker 1977)
   3.69   (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
   3.70   (from activity coefficient measurement, Berti et al. 1986)
   3.44   (recommended, Sangster 1989, 1993)
   3.73   (from activity coefficient measurement, Tse & Sandler 1994)
   3.44   (recommended, Hansch et al. 1995)

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

   2.83*   (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
   2.71   (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

   2.38   (estimated, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

   2.68   (estimated-S, Howard 1990)

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

   Volatilization: $t_{1/2}$ = 2.8 h from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982, quoted, Howard 1990).
   Photolysis:
   Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
      k_{OH}*(exptl) = 5.38 × 10^{12} cm^3 mol^{-1} s^{-1}, k_{OH}(calc) = 4.79 × 10^{12} cm^3 mol^{-1} s^{-1} at 295 K, measured range 295–497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
      k_{OH} (exptl) = 6.7 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K; k_{OH} (calc) = 6.7 × 10^{-12} cm^3·molecule^{-1}s^{-1} at 300 K (Darnall et al. 1978)
      $k_{O(3P)}$ = 1.40 × 10^{-13} cm^3·molecule^{-1} s^{-1} for the reaction with O(^{3}P) atoms at room temp. (Herron & Huie 1973)
      k_{OH} = 7.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)
      k_{OH} = (7.57 ± 0.05) × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = (6.20 \pm 0.44) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at $(24.4 \pm 0.4)°$C with an atmospheric lifetime of 1.9 d for an average OH radical concentration of 1.0×10^6 molecules/cm^3 (Edney et al. 1986)

$k_{OH} = 7.34 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

$k_{OH} = 7.14 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 292 K, measured range 292–491 K (Droege & Tully 1987)

$k_{OH} = 7.38 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Dilling et al. 1988)

$k_{OH}* = 7.49 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH}* = 7.49 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, $k_{NO3} = 13.4 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)

$k_{NO3} = 1.35 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1991)

k_{NO3}(exptl) $= 1.35 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, k_{NO3}(calc) $= 2.04 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}* = 7.21 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

$k_{OH}* = 6.69 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation: highly resistant to biodegradation (Howard 1990);

$t_{1/2}$(aq. aerobic) = 672 to 4032 h, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991);

$t_{1/2}$(aq. anaerobic) = 2688 to 16280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim$ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

atmospheric lifetime τ = 1.9 d for an average OH radical concentration of 1.0×10^6 molecules/cm^3 (Edney et al. 1986);

$t_{1/2}$ = 52 h, based on photooxidation rate constant (Howard 1990);

an atmospheric lifetime $\tau \sim$ 19 h in summer daylight, based on the photooxidation reaction rate constant of 7.49×10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with OH radical in air during summer daylight (Altshuller 1991);

will degrade photochemically by hydroxyl radicals with $t_{1/2}$ = 52 h and much faster under photochemical smog conditions with $t_{1/2}$ = 6 h (Howard 1990);

$t_{1/2}$ = 8.7 - 87 h, based on reaction with OH radical half-life in air (Howard et al. 1991).

Surface water: volatilization $t_{1/2}$ = 2 h in a model river (Howard 1990);

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

photooxidation $t_{1/2} = 1.4 \times 10^9$ to 6.9×10^{10} h (16000 to 780000 yr), based on measured rate data for alkylperoxyl radicals in aqueous solution (Howard et al. 1991).

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

Sediment:

Soil: $t_{1/2}$ = 672–4320 h, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991).

Biota:

TABLE 2.1.1.2.6.1
Reported aqueous solubilities of cyclohexane at various temperatures

Pierotti & Liabastre 1972		Tsonopoulos & Wilson 1983		Shaw 1989a	
shake flask-GC		shake flask-GC		IUPAC recommended	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	S/g·m⁻³
5.11	81.93	40	72.8	5	-
15.21	88.70	100	1770	15	-
25.11	88.84	146.89	4810	20	-
35.21	88.84	150	6070	25	58.0
45.21	91.32	200	18300	45	-
		209.06	23000	50	-
				56	-
				70	-
				71	-
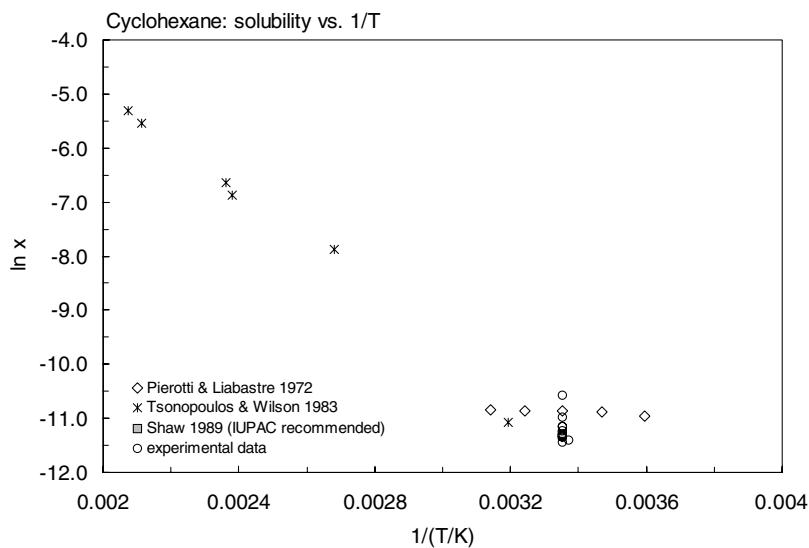
FIGURE 2.1.1.2.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for cyclohexane.

TABLE 2.1.1.2.6.2
Reported vapor pressures of cyclohexane at various temperatures and the coefficients for the vapor pressure equations:

$$\log P = A - B/(T/K) \qquad (1)$$
$$\ln P = A - B/(T/K) \qquad (1a)$$
$$\log P = A - B/(C + t/°C) \qquad (2)$$
$$\ln P = A - B/(C + t/°C) \qquad (2a)$$
$$\log P = A - B/(C + T/K) \qquad (3)$$
$$\log P = A - B/(T/K) - C·\log (T/K) \qquad (4)$$
$$\log P = A - B/(T/K) - C·\log (T/K) + D[P/(T/K)^2] \qquad (5)$$
$$\log P = A - B/T(T/K) - C/(T/K)^2 \qquad (6)$$

1.

Ashton et al. 1943b		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
manometry		ebulliometry		summary of literature data		selected exptl. data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
6.33	5388	19.915	10303	−45.3	133.3	20.015	10253
9.89	6421	22.657	11695	−25.4	666.6	52.693	39997
13.63	7697	26.347	13821	−15.9	1333	82.469	106658
17.65	9327	30.556	16610	−5.0	2666	105.215	199984
20.97	10910	34.821	19917	6.7	5333	160.015	670345
		38.789	23453	14.7	7999	219.905	1813184
mp/°C	6.69	44.108	28960	25.5	13332	240.395	3420467
bp/°C	80.8	48.991	43324	42.0	26664	278.075	3959408
		54.884	53659	60.8	53329		
$\Delta H_v/(kJ\ mol^{-1})$ = 33.33		60.969	66762	80.7	101325	bp/°C	80.75
at 25°C		67.467	83723				
$\Delta H_{fus}/(kJ\ mol^{-1})$ = 2.627		74.520	97609	mp/°C	6.60	Frost-Kalkwarf equation	
		79.052	99209			derived from exptl. data	
		80.037	100701			eq. 5	P/mmHg
		80.534	102403			A	23.14002
Scatchard et al. 1939		81.093	103923			B	−2411.8
vapor-liquid equilibrium		81.582	103923			C	−5.27900
t/°C	P/Pa					D	1.84394
30	16212	bp/°C	80.738			Frost-Kalkwarf equation	
40	24613	eq. 2	P/mmHg			calculated from molecular	
50	36237	A	6.84498			structures, normal bp and	
60	51901	B	1203.526			deviations of resulting v.p.	
70	72521	C	222.863			eq. 5	P/mmHg
80	88995					A	23.09550
						B	−2411.82
eq. 6	P/mmHg					C	−5.26151
A	6.65859					D	1.84394
B	1040.641						
C	116.197						

(Continued)

2.

Boublik 1960		Cruickshank & Cutler 1966		Zwolinski & Wilhoit 1971		Ewing & Ochoa 2000	
in Boublik et al. 1984		static method-manometry		selected values		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
17.55	9210	25	13040	6.69	5333	8.188	5777
20.16	10426	35	20104	11.01	6666	9.698	6243
22.98	11876	45	30008	14.66	7999	11.356	6791
25.26	13159	55	43538	20.666	10666	15.215	8225
28.77	15372	65	61551	25.536	13332	17.163	9039
32.77	18252	75	85012	34.904	19998	19.868	10284
37.10	21891			41.991	26664	22.608	11675
40.66	25264	mp/°C	6.55	47.763	33331	23.263	12086
45.77	30864	bp/°C	80.728	52.669	39997	28.346	15109
50.96	37543	density, d^{25}	0.77386	60.784	53329	44.379	29290
56.18	45356			67.415	66661	49.393	35456
62.46	56448	$\Delta H_V/(kJ\ mol^{-1}) =$		73.067	79993	55.302	44015
68.71	69467	at 20°C	33.23	78.021	93326	60.881	53541
75.42	86053	25°C	32.97	78.944	95992	66.269	64227
80.22	99818	54.1°C	31.45	79.848	98659	71.034	75023
		73.3°C	30.44	80.292	99992	75.094	86306
bp/°C	80.731	80.7°C	30.03	80.732	101325	78.498	94753
						80.80	101589
		eq. 2	P/mmHg	eq. 2	P/mmHg	83.489	110504
		A	6.85875	A	6.84130	87.149	122451
		B	1212.014	B	1201.531		
		C	233.956	C	222.647		
				bp/°C	80.732	temp range 281–552 K	
				$\Delta H_V/(kJ\ mol^{-1}) =$		data fitted to Wagner eq.	
				at 25°C	33.04		
				at bp	29.96		

FIGURE 2.1.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexane.

TABLE 2.1.1.2.6.3
Reported Henry's law constants and octanol-air partition coefficients of cyclohexane 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)		
$\ln [H/(Pa \cdot m^3/mol)] = A - B/(T/K)$ (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)		

Henry's law constant				log K_{OA}	
Ashworth et al. 1988		Kolb et al. 1992		Gruber et al. 1997	
EPICS-GC		equilibrium headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
10	10436	40	37190	20.29	2.835
15	12767	60	55400	30.3	2.652
20	14189	70	95100	40.4	2.511
25	17935	80	146800	50.28	2.365
30	22595				
		eq. 2	1/K_{AW}		
		A	−12.90		
eq. 4a	H/(atm m³/mol)	B	−3228		
A	9.141				
B	3238				
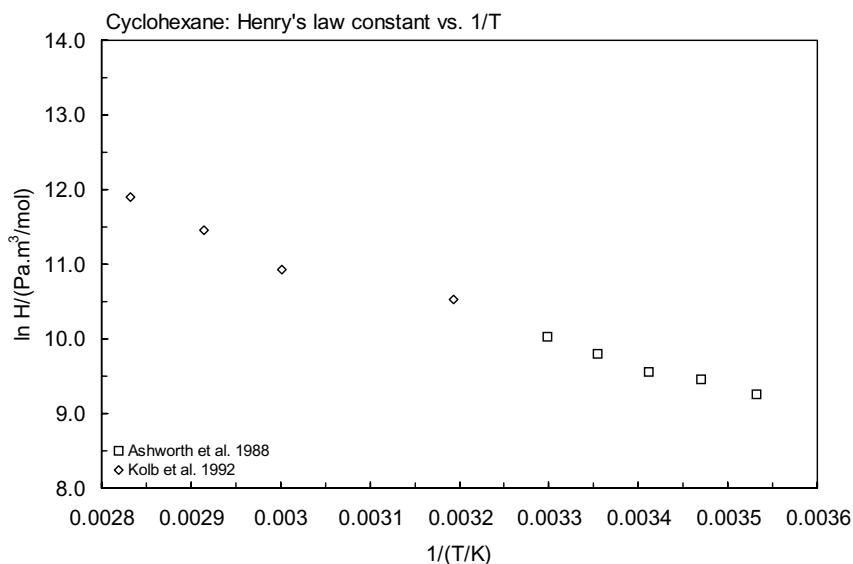
FIGURE 2.1.1.2.6.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclohexane.
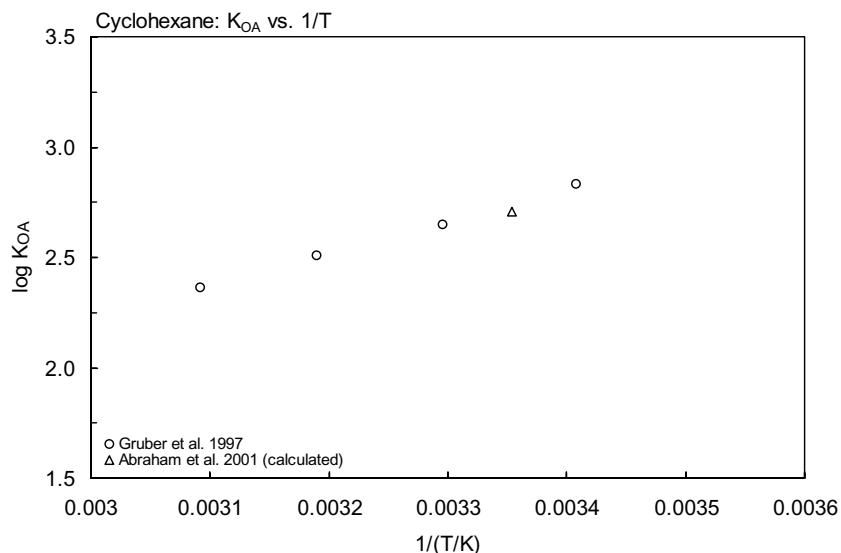
FIGURE 2.1.1.2.6.4 Logarithm of K_{OA} versus reciprocal temperature for cyclohexane.

2.1.1.2.7   Methylcyclohexane
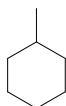
Common Name: Methylcyclohexane
Synonym: hexahydrotoluene, cyclohexylmethane
Chemical Name: methylcyclohexane
CAS Registry No: 108-87-2
Molecular Formula: C_7H_{14}
Molecular Weight: 98.186
Melting Point (°C):
     –126.6   (Dreisbach 1959; Weast 1984; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
     100.93   (Lide 2003)
Density (g/cm³ at 20°C):
     0.7694, 0.7651 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm³/mol):
     127.6   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
     140.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     35.359, 31.13 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     6.757   (Riddick et al. 1986)
     6.75   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     46.1, 47.3 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
     data at other temperatures designated * are compiled at the end of this section.):
     14.0   (shake flask-GC, McAuliffe 1963, 1966)
     16.0*   (shake flask-GC, measured range 25–149.5°C, Price 1976; quoted, Eastcott et al. 1988)
     15.3   (partition coefficient-GC, Rudakov & Lutsyk 1979)
     15.2   (20°C, shake flask-GC, Burris & MacIntyre 1986)
     16.7   (shake flask-GC, Groves 1988)
     15.1*   (IUPAC recommended, temp range 25–150°C, Shaw 1989)
     15.82*   (calculated-liquid-liquid equilibrium LLE data, temp range 298.2–410.5 K, Mączyński et al. 2004)
     16.15*   (26.1°C, shake flask-GC, measured range 26.1–170.8°C, Marche et al. 2004)
     ln (S/ppm) = 13.091 – 7085.522/(T/K) + 1055594/(T/K)² (Marche et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
     temperatures designated * are compiled at the end of this section.):
     6128   (interpolated-Antoine eq., Stuckey & Saylor 1940)
     log (P/mmHg) = 6.95423 – 1336.93/(T/K – 45.52); temp range 4–75°C (Antoine eq. based on exptl. data,
          Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)
     6354*   (25.59°C, ebulliometry-manometer, Willingham et al. 1945)
     log (P/mmHg) = 6.82689 – 1272.864/(221.630 + t/°C); temp range 25.6–101.8°C (Antoine eq. from exptl. data,
          ebulliometry-manometer, Willingham et al. 1945)
     5887*   (calculated-Antoine eq. regression, temp range –35.9 to 100.0°C, Stull 1947)
     6180   (calculated from determined data, Dreisbach 1955)
     log (P/mmHg) = 6.82689 – 1272.864/(221.630 + t/°C); temp range 10–155°C (Antoine eq. for liquid state,
          Dreisbach 1955)
     10207*   (35.901°C, temp range 35.901–95.946°C, Varushchenko et al. 1970)

6180*   (interpolated-Antoine eq., temp range –3.20 to 127.0°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.82300 – 1272.763/(221.416 + t/°C); temp range –3.20 to 127.0°C (Antoine eq., Zwolinski & Wilhoit 1971)

5880   (interpolated-Antoine eq., temp range –35.9 to 100°C, Weast 1972–73)

log (P/mmHg) = [–0.2185 × 8549.2/(T/K)] + 7.909762; temp range –35.9 to 100°C (Antoine eq., Weast 1972–73)

5806   (calculated-bp, Mackay et al. 1982)

log (P/atm) = [1– 373.957/(T/K)] × 10^{0.862568 – 8.71426 × 10^{-4}·(T/K) + 8.69685 × 10^{-7}·(T/K)^2}; temp range 203.20–563.20 K (Cox eq., Chao et al. 1983)

5364, 6111, 6177 (Antoine equations, Boublik et al. 1984)

log (P/kPa) = 5.95366 – 1273.962/(221.755 + t/°C); temp range 25.6–101.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 5.95497 – 1275.047/(221.678 + t/°C); temp range 35.9–95.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.92856 – 1253.199/(216.058 + t/°C); temp range 58.645–113.6°C (Antoine eq. from reported exptl. data of Meyer et al. 1976, Boublik et al. 1984)

6180   (interpolated-Antoine eq., temp range –3 to 127°C, Dean 1985, 1992)

log (P/mmHg) = 6.82300 – 1270.763/(221.42 + t/°C); temp range –3 to 127°C (Antoine eq., Dean 1985, 1992)

6100   (quoted lit., Riddick et al. 1986)

log (P/kPa) = 5.94790 – 1270.763/(221.416 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

6160   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.9428 – 1266.954/(–52.282 + T/K); temp range 308–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.14677 – 1413.495/(–32.726 + T/K); temp range 373–511 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.29186 – 2700.205/(147.549 + T/K); temp range 501–573 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 38.0955 – 3.0738 × 10^3/(T/K) –10.684·log (T/K) – 5.1766 × 10^{-11}·(T/K) + 3.5282 × 10^{-6}·(T/K)^2; temp range 147–572 K (vapor pressure eq., Yaws 1994)

5205*   (21.46°C, static method-manometry, measured range –76.96 to 41.44°C, Mokbel et al. 1995)

ln x = –328.666 + 14073.29/(T/K) + 47.1467·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)

ln x = –491.070 + 22132.10/(T/K) + 70.9150·ln (T/K); temp range 290–400 K (eq. derived from direct fit of solubility data, Tsonopoulos 2001)

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.):

44080   (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

31030, 41340   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

40000   (recommended; Mackay & Shiu 1981)

31934   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

37930   (calculated-P/C, Eastcott et al. 1988)

43300   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

12666*   (27.3°C, EPICS-GC, measured range 27.3–45°C, Hansen et al. 1993)

ln [H/(kPa·m^3/mol)] = –9406/(T/K) + 34.0; temp range 27.3–45°C (EPICS-GC, Hansen et al. 1993)

6410   (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 13.507 – 3836/(T/K) (summary of literature data, Staudinger & Roberts 2001)

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

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

2.96   (calculated- MCI π, Murray et al. 1975)

2.82   (Hansch & Leo 1979)

3.88   (recommended, Sangster 1989. 1993)

4.10   (calculated-fragment const. per Lyman 1982, Thoms & Lion 1992)

2.89   (calculated-molar volume V_M, Wang et al. 1992)

3.87   (calculated-fragment const., Müller & Klein 1992)
3.61   (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated *
    are compiled at the end of this section:
    3.14*   (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C Gruber et al. 1997)
    3.05   (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k 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:
        $k_{OH} = (10.6 \pm 0.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)
        $k_{OH} = 1.04 \times 10^{-11}$ cm^3·molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)
        $k_{OH} = 1.04 \times 10^{-11}$ cm^3·molecule^{-1} s^{-1} at 298 K with an estimated half-life of 13 h (Altshuller 1991)
        $k_{OH} = 1.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biotransformation:
    Biodegradation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
    Air: an atmospheric lifetime was estimated to be 13 h in summer daylight, based on the photooxidation rate
        constant of 1.04×10^{-11} cm^3 molecule^{-1} s^{-1} with hydroxyl radicals in air (Altshuller 1991).

TABLE 2.1.1.2.7.1
Reported aqueous solubilities of methylcyclohexane at various temperatures

Price 1976		Shaw 1989a		Marche et al. 2004		Mączyński et al. 2004	
Shake flask-GC		IUPAC recommended		Shake flask-GC		Calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
		25	15.1	26.1	16.15	25	15.82
25.0	16.0	30	17.0	70.5	27.49	40.1	16.91
40.1	18.0	40	18.0	100.5	54.88	55.7	19.64
55.7	18.9	50	19.0	131.0	133.1	99.1	44.18
99.1	33.8	70	22.0	151.4	230.7	120	76.37
120.0	79.5	90	29.0	170.8	386.2	137.3	125.5
137.3	139	110	52.0				
149.5	244	130	110	$S = A - B/(T/K) + C/(T/K)^2$			
		150	250	S	g/m^3		
				A	13.091		
				B	7085.522		
				C	1055594		

FIGURE 2.1.1.2.7.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.2
Reported vapor pressures of methylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$	(3)	
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D[P/(T/K)^2]$	(5)	

1.

Willingham et al. 1945		Stull 1947		Varushchenko et al. 1970		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.585	6354	−35.9	133.3	35.901	10207	−3.20	1333
29.533	7655	−14.0	666.6	45.809	15552	8.70	2666
32.976	8962	−3.2	1333	50.799	19018	16.3	4000
36.089	10303	8.7	2666	55.419	22754	21.98	5333
38.998	11696	22.0	5333	61.644	28719	26.585	6666
42.929	13820	35.0	7999	67.476	35390	30.477	7999
47.407	16919	42.1	13332	74.177	44530	36.874	10666
51.964	19918	59.6	26664	81.020	55721	42.063	13332
56.194	23453	79.6	53329	88.101	69542	52.048	19998
61.857	28958	100.0	101325	93.567	81944	59.604	26664
67.067	34896			94.159	93376	65.758	33331
73.349	43323	mp/°C	−126.4	94.766	84890	70.990	39997
79.842	53657			95.307	86243	79.646	53329
86.771	66760			95.946	87847	86.720	66661
94.299	83721					92.752	79993
99.614	97628					98.039	93326
100.185	99205					99.025	95992
100.715	100697					99.989	98659
101.312	102398					100.464	99992
101.832	103919					100.934	101325

TABLE 2.1.1.2.7.2 *(Continued)*

Willingham et al. 1945		Stull 1947		Varushchenko et al. 1970		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
100.715	100697					99.989	98659
101.312	102398					100.464	99992
101.832	103919					100.934	101325
bp/°C	100.934					eq. 2	P/mmHg
						A	6.82300
eq. 2	P/mmHg					B	1270.763
A	6.82689					C	221.416
B	1272.864					bp/°C	100.934
C	221.630					$\Delta H_V/(kJ\ mol^{-1}) =$	
						at 25°C	35.36
						at bp	31.13

2.

Mokbel et al. 1995						
static method-manometry						
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
−76.96	1.68	−28.28	240	21.46	5205	
−67.0	5.87	−18.38	497	31.45	8368	
−58.55	15.8	−8.44	970	41.44	12950	
−48.64	42.4	1.50	1785			
−38.15	108	11.47	3128	data fitted to Wagner eq.		
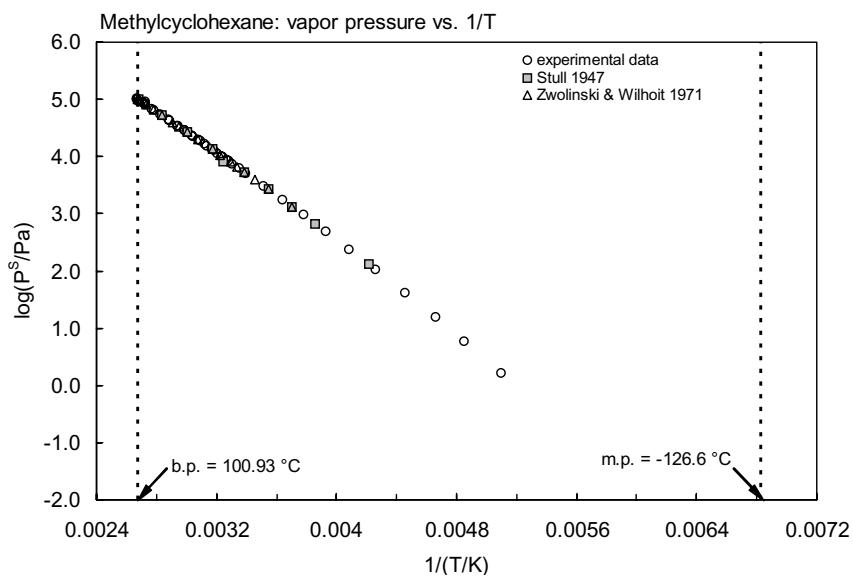
FIGURE 2.1.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.3
Reported Henry's law constants and octanol-air partition coefficients of methylcyclohexane 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)		

Henry's law constant		log K_{OA}	
Hansen et al. 1993		Gruber et al. 1997	
EPICS-GC		GC det'd activity coefficient	
t/°C	H/(kPa m³/mol)	t/°C	.log K_{OA}
27.3	12.666	20.29	3.142
35.8	34.653	30.3	2.943
45.0	72.447	40.4	2.784
		50.28	2.632
eq. 4	H/(kPa m³/mol)		
A	34 ± 3.39		
B	9406 ± 1046		
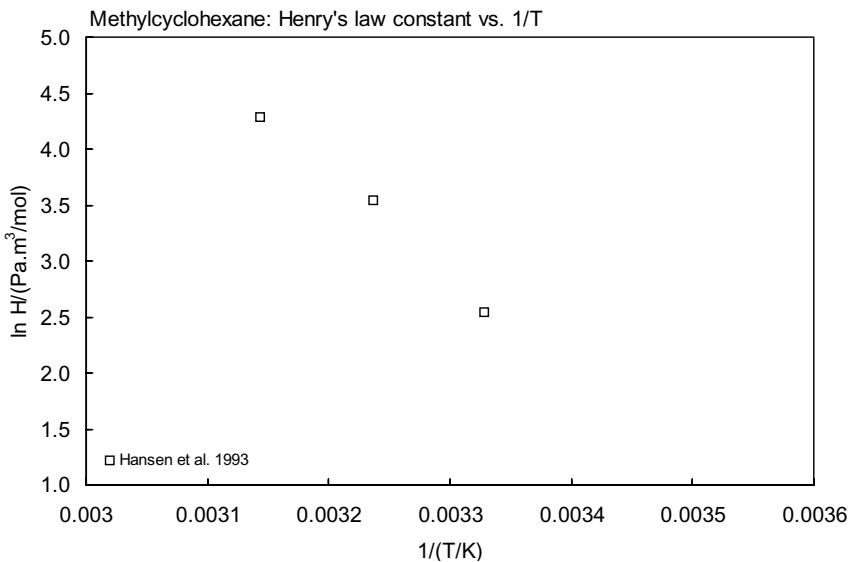
FIGURE 2.1.1.2.7.3 Logarithm of Henry's law constant versus reciprocal temperature for methylcyclohexane.
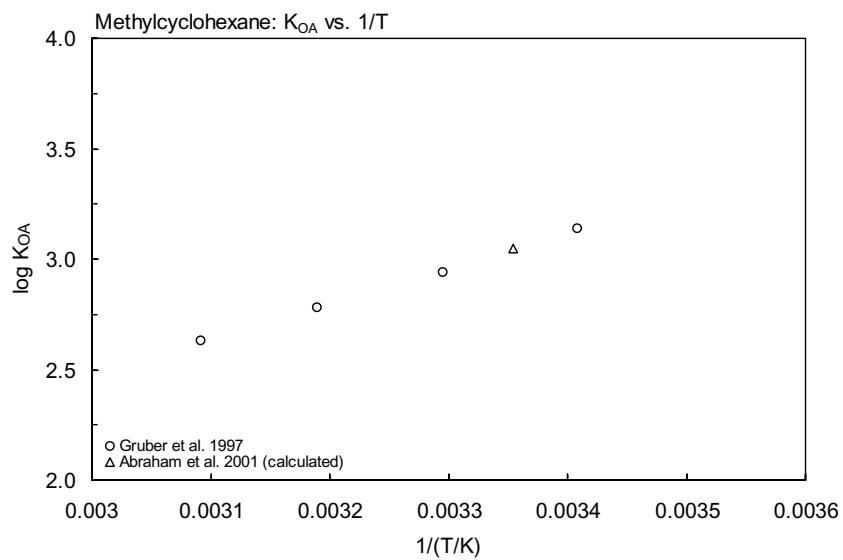
FIGURE 2.1.1.2.7.4 Logarithm of K_{OA} versus reciprocal temperature for methylcyclohexane.

2.1.1.2.8   *1,2,-cis-Dimethylcyclohexane*
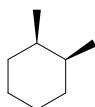
Common Name: 1,2-*cis*-Dimethylcyclohexane
Synonym: *cis*-1,2-dimethylcyclohexane
Chemical Name: 1,2-*cis*-dimethylcyclohexane
CAS Registry No: 2207-01-4
Molecular Formula: C_8H_{16}
Molecular Weight: 112.213
Melting Point (°C):
    –49.8   (Lide 2003)
Boiling Point (°C):
    129.8   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7963, 0.7922   (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm³/mol):
    140.9   (20°C, calculated-density, McAuliffe 1966)
    141.6   (25°C, calculated-density; Ruelle & Kesselring 1997)
    162.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    39.715, 34.196 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    1.644   (Dreisbach 1955; Riddick et al. 1986)
    8.26, 1.64   (–100.65, –39.05°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    55.22, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    6.0   (shake flask-GC, McAuliffe 1966)
    5.01   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)
    5.94*   (generator column-GC, measured range 273.15–313.15 K, Dohányosová et al. 2004)
    ln x = –59.7348 + 45.8700/τ + 46.6282·ln τ; τ = T/298.15 K (empirical eq., generator column-GC, Dohányosová
        et al. 2004)
    ln (S/ppm) = 11.610 – 8455.943/(T/K) + 961943.2/(T/K)², temp range 30.3–170°C (Marche et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    6352*   (49.185°C, ebulliometry, measured range 49.185–130.684°C, Willingham et al. 1945)
    1333*   (18.4°C, summary of literature data, temp range –15.9 to 129.7°C, Stull 1947)
    log (P/mmHg) = 6.84164 – 1369.525/(216.040 + t/°C); temp range 49.2–130.7°C (Antoine eq. from exptl. data,
        ebulliometry-manometer, Willingham et al. 1945)
    1929   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 6.84164 – 1369.525/(216.040 + t/°C); temp range 40–170°C (Antoine eq. for liquid state,
        Dreisbach 1955)
    1933*   (interpolated-Antoine eq., temp range 18.4–157.6°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.83746 – 1367.311/(215.835 + t/°C); temp range 18.4–157.6°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 9364.9/(T/K)] + 8.001159; temp range –15.9 to 129.7°C (Antoine eq., Weast
        1972–73)

log (P/atm) = [1– 402.894/(T/K)] × 10^{0.841813 – 8.56119 × 10^{-4}·(T/K) + 5.01855 × 10^{-7}·(T/K)^2}; temp range: 257.25–430.75 K (Cox eq., Chao et al. 1983)

1927   (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.96885 – 1370.962/(216.202 + t/°C); temp range 49.2–130.68°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

1928   (interpolated-Antoine eq., temp range 18–158°C, Dean 1985, 1992)

log (P/mmHg) = 6.83746 – 1367.311/(215.84 + t/°C); temp range 18–158°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 5.96654 – 1369.525/(216.040 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P$_L$/kPa) = 5.96232 – 1367.306/(–57.314 + T/K); temp range 322–405 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 32.1535 – 3.0728 × 10^3/(T/K) – 8.4344·log (T/K) + 6.8943 × 10^{-10}·(T/K) + 1.9558 × 10^{-6}·(T/K)^2; temp range 223–606 K (vapor pressure eq., Yaws 1994)

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

36000   (calculated-P/C, Mackay & Shiu 1981)

35830   (calculated-1/K$_{AW}$, C$_W$/C$_A$, reported as exptl., Hine & Mookerjee 1975)

53000, 62270   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

44080   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

36045   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

36180*   (derived from solute fugacity and mole fraction solubility, temp range 273.15–313.15 K, Dohányosová et al. 2004)

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

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

3.33   (calculated-MCI χ, Murray et al. 1975)

3.21   (calculated-molar volume V$_M$, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

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

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

Half-Lives in the Environment:

Air: atmospheric t$_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.8.1
Reported aqueous solubilities and Henry's law constants of 1,2-*cis*-dimethylcyclohexane at various temperatures

Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC/FID		smoothed raw exptl data		from solute fugacity f and x	
T/K	S/g·m⁻³	T/K	S/g·m⁻³	T/K	H/(Pa m³/mol)
	raw data				
274.15	6.608	273.15	6.59	273.15	7218
274.15	6.670	278.15	6.27	278.15	10566
274.15	6.421	283.15	6.05	283.15	14994
278.15	6.184	288.15	5.93	288.15	20700
278.15	6.234	293.15	5.90	293.15	27720
278.15	6.078	298.15	5.94	298.15	36180
283.75	6.159	303.15	6.06	303.15	46260
283.75	6.041	308.15	6.25	308.15	57780
288.15	5.767	313.15	6.51	313.15	70740
288.15	6.234				
288.15	6.147	$\ln x = A + B/\tau + C \ln \tau$			
293.15	5.960	$\tau = T/298.15$			
293.15	5.679	A	−59.7348		
293.15	5.980	B	45.8700		
298.15	5.979	C	46.6282		
298.15	5.866				
298.15	6.003	$\Delta H_{sol}/(kJ\ mol^{-1})$			
303.15	6.190	25°C			
308.15	6.483				
308.15	6.016				
313.15	6.546				
313.15	6.483				
313.15	6.795				
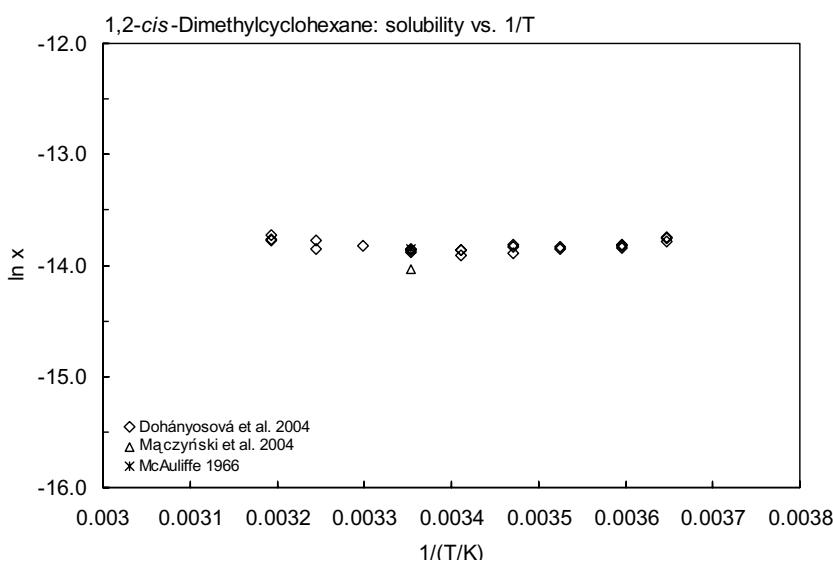
FIGURE 2.1.1.2.8.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.
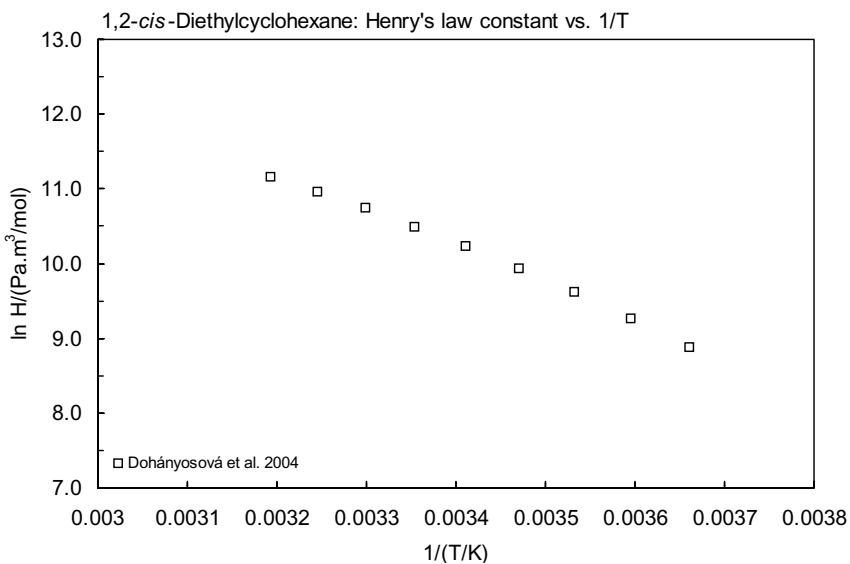
FIGURE 2.1.1.2.8.2 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.

TABLE 2.1.1.2.8.2
Reported vapor pressures of 1,2-*cis*-dimethylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \qquad (1)$$
$$\log P = A - B/(C + t/°C) \qquad (2)$$
$$\log P = A - B/(C + T/K) \qquad (3)$$
$$\log P = A - B/(T/K) - C·\log (T/K) \qquad (4)$$
$$\ln (P/P_{ref}) = [1 - (T_{ref}/T)]·\exp(a + bT + cT^2) \qquad (5)$$

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

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
49.185	6352	−15.9	133.3	18.4	1333
53.413	7655	7.30	666.6	31.1	2666
57.094	8966	18.4	1333	39.24	4000
60.429	10304	31.1	2666	45.33	5333
63.543	11696	45.3	5333	50.257	6666
67.742	13820	54.4	7999	54.421	7999
72.553	16608	66.8	13332	61.264	10666
77.402	19924	85.6	26664	66.815	13332
81.921	23451	107.0	53329	77.493	19998
87.974	28955	129.7	101325	85.572	26664
93.548	34897			92.151	33331
100.258	43324	mp/°C	−50	97.744	39997
107.192	53656			106.944	53329
114.600	66759			114.554	66661
122.639	83718			120.998	79993
128.315	97607			126.647	93326
128.926	99203			127.699	95992
129.491	100694			128.729	98659
130.125	102389			129.738	101325

(Continued)

TABLE 2.1.1.2.8.2 *(Continued)*

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
130.684	103909			25.0	1933
bp/°C	124.450			eq. 2	P/mmHg
				A	6.83746
eq. 2	P/mmHg			B	1367.311
A	6.83866			C	215.835
B	1345.859			bp/°C	129.738
C	215.598			ΔH_V/(kJ mol^{-1}) =	
temp range 45.2–125.4°C				a 25°C	39.71
pressure range 48–780 mmHg				a bp	33.64
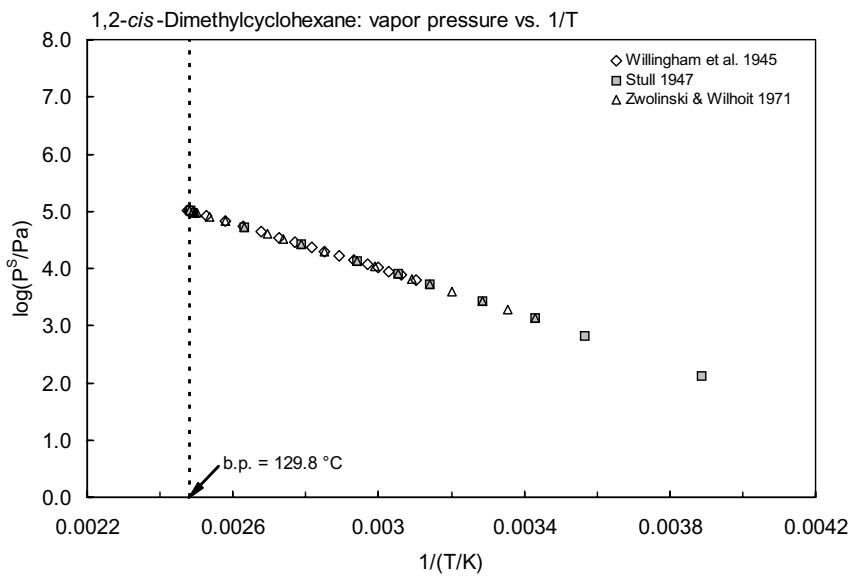
FIGURE 2.1.1.2.8.3 Logarithm of vapor pressure versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.

*2.1.1.2.9   1,4-*trans-*Dimethylcyclohexane*
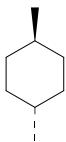
Common Name: 1,4-*trans*-Dimethylcyclohexane
Synonym: *trans*-1,4-dimethylcyclohexane
Chemical Name: 1,4-*trans*-dimethylcyclohexane
CAS Registry No: 2207-04-7
Molecular Formula: C_8H_{16}
Molecular Weight: 112.213
Melting Point (°C):
    –36.93   (Lide 2003)
Boiling Point (°C):
    119.4   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7626, 0.7584   (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
    147.2, 148   (20°C, 25°C, calculated-density)
    162.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    38.14, 33.05 (25°, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    11.422   (Dreisbach 1955)
    12.34   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    52.26, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

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

    3.84   (shake flask-GC, Price 1976; quoted, Shaw 1989)

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

    log (P/mmHg) = 6.82180 – 1332.613/(218.791 + t/°C); temp range 40.3–120.3°C (Antoine eq. from exptl. data,
        ebulliometry-manometer, Willingham et al. 1945)
    3025   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 6.82180 – 1332.613/(218.791 + t/°C); temp range 30–155°C (Antoine eq. for liquid state,
        Dreisbach 1955)
    3026   (interpolated-Antoine eq., temp range 10.1–146.8°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.81773 – 1330.437/(218.581 + t/°C); temp range 10.1–146.8°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 8951.2/(T/K)] + 7.898079; temp range –24.3 to 119.5°C (Antoine eq., Weast
        1972–73)
    log (P/atm) = [1– 396.346/(T/K)] × 10^{0.827486 – 6.12608 × 10⁻⁴·(T/K) + 4.53086 × 10⁻⁷·(T/K)²}; temp range:
        252.05–424.25 K (Cox eq., Chao et al. 1983)
    3024   (interpolated-Antoine eq., temp range 10–147°C, Dean 1985, 1992)
    log (P/mmHg) = 6.81773 – 1330.437/(218.58 + t/°C); temp range 10–147°C (Antoine eq., Dean 1985, 1992)
    log (P_L/kPa) = 5.94449 – 1331.612/(–54.43 + T/K); temp range 313–395 K (Antoine eq., Stephenson &
        Malanowski 1987)
    log (P/mmHg) = 32.5731 – 2.9872 × 10³/(T/K) – 8.6494·log (T/K) – 2.1355 × 10⁻⁹·(T/K) + 2.2946 × 10⁻⁶·(T/K)²;
        temp range 236–590 K (vapor pressure eq., Yaws 1994)

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

    88200   (calculated-P/C, Mackay & Shiu 1981)

    88360   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

    Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

2.1.1.2.10   1,1,3-Trimethylcyclohexane
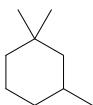
Common Name: 1,1,3-Trimethylcyclohexane
Synonym:
Chemical Name: 1,1,3-trimethylcyclohexane
CAS Registry No: 3073-66-3
Molecular Formula: C_9H_{18}
Molecular Weight: 126.239
Melting Point (°C):
        –65.7   (Lide 2003)
Boiling Point (°C):
        136.6   (Lide 2003)
Density (g/cm³ at 20°C): 0.7664
Molar Volume (cm³/mol):
        164.7   (20°C, calculated-density, Ruelle & Kesselring 1997)
        184.8   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
        1.77   (shake flask-GC, Price 1976)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    log (P/mmHg) = 6.83705 – 1393.299/(215.551 + t/°C); temp range 54.7–137.6°C (Antoine eq., ebulliometry-
        manometer measurements, Forziati et al. 1949)
    log (P/atm) = [1– 409.802/(T/K)] × 10^{0.838270 – 6.63916 × 10^{-4}·(T/K) + 5.61172 × 10^{-7}·(T/K)²}; temp range:
        327.82–410.80 K (Cox eq., Chao et al. 1983)
    1480   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.96492 – 1395.206/(215.77 + t/°C); temp range 54.67–137.6°C (Antoine eq. from reported exptl.
        data of Forziati et al. 1949, Boublik et al. 1984)
    log (P/kPa) = 5.96816 – 1397.161/(215.961 + t/°C); temp range 54.69–137.65°C (Antoine eq. from reported
        exptl. data of Pasek & Thodos 1962, Boublik et al. 1984)
    1480   (interpolated-Antoine eq., temp range 55–137°C, Dean 1985, 1992)
    log (P/mmHg) = 6.83951 – 1394.88/(215.73 + t/°C); temp range 55–137°C (Antoine eq., Dean 1985, 1992)
    log (P_L/kPa) = 5.96449 – 1395.396/(–57.308 + T/K); temp range 348–411 K (Antoine eq., Stephenson &
        Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):
    105600   (calculated-P/C from selected data)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: 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:
        $k_{OH} = 8.73 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (Atkinson 1989)
        $k_{OH} = 8.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.2.11   Ethylcyclohexane
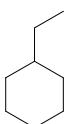
Common Name: Ethylcyclohexane
Synonym:
Chemical Name: ethylcyclohexane
CAS Registry No: 1678-91-7
Molecular Formula: C_8H_{16}, $C_2H_5C_6H_{11}$
Molecular Weight: 112.213
Melting Point (°C):
    −111.3   (Weast 1982–83; Lide 2003)
Boiling Point (°C):
    131.9   (Lide 2003)
Density (g/cm³):
    0.7880   (20°C, Weast 1982–82)
Molar Volume (cm³/mol):
    142.4   (20°C, calculated-density, Stephenson & Malanowski 1987)
    162.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    7.0*   (40°C, shake flask-solid phase extraction-GC, measured range 38.35–280°C, Heidman et al. 1985)
    $\ln x = -334.2468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K)$; measured range 40–280°C (shake flask-solid phased
        extraction-GC, Heidman et al. 1985)
    7.0*   (40°C, IUPAC tentative value, temp range 40–280°C, Shaw 1989a)
    3.89*   (generator column-GC/FID, measured range 273.15–313.15 K, Dohányosová et al. 2004)
    $\ln x = -53.6687 + 39.4055/\tau + 41.1210 \cdot \ln \tau$, $\tau = [(T/K)/298.15]$, temp range 273.15–313.15 K (generator column-
        GC/FID, Dohányosová et al. 2004)
    4.36*   (30.3°C, shake flask-GC, measured range 30.3–170.8°C, Marche et al. 2004)
    $\ln x = -344.02468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K)$; temp range 30.3–170.8°C (Marche et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    6351*   (51.412°C, ebulliometry, measured range 51.4–132.7°C, Willingham et al. 1945)
    1612   (extrapolated-Antoine eq., Willingham et al. 1945)
    $\log (P/mmHg) = 6.87041 - 1384.036/(214.128 + t/°C)$; temp range 51.4–132.7°C (Antoine eq., ebulliometry,
        Willingham et al. 1945)
    1333*   (20.6°C, summary of literature data, temp range −14.5 to 131.9°C, Stull 1947)
    1705*   (extrapolated-Antoine eq., temp range 20.6–159.5°C, Zwolinski & Wilhoit 1971)
    $\log (P/mmHg) = 6.86728 - 1382.466/(214.995 + t/°C)$; temp range 20.6–159.5°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    $\log (P_L/kPa) = 5.99043 - 1381.396/(-58.271 + T/K)$; temp range 323–407 K (Antoine eq., Stephenson &
        Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C Additional data at other temperatures designated * are compiled at the end of this section.):

ln (k_H/MPa) = 325.570 – 18496.5/(T/K) – 10.9666·(T/K)² – 44.7690·ln (T/K); maximum k_H = 1.186 × 10⁴ MPa at 385.2 K (Heidman et al. 1985)

48960*   (derived from solute fugacity and mole fraction solubility, temp range 273.15–323.15 K, Dohányosová et al. 2004)

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

TABLE 2.1.1.2.11.1
Reported aqueous solubilities of ethylcyclohexane at various temperatures

ln x = A + B/(T/K) + C ln (T/K)   (1)

Heidman et al. 1985		Shaw 1989a		Dohányosová et al. 2004		Marche et al. 2004	
shake flask-GC		IUPAC "tentative" best		generator column-GC		shake flask-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	T/K	S/g·m⁻³	t/°C	S/g·m⁻³
38.35	6.8	40	7.0	274.15	3.803	30.3	4.358
94.45	15.0	50	7.0	274.15	4.108	70.4	8.790
150.25	120	60	7.0	278.15	3.996	100.5	28.18
206.35	750	70	10	278.15	3.678	131.0	67.95
263.15	7300	80	13	283.15	3.734	151.2	110.8
279.65	14600	90	16	288.15	3.759	170.8	183.3
		100	21	288.15	3.666		
eq. 1	x	120	55	293.15	3.766		
A	–334.2468	140	95	293.15	3.797		
B	14105.21	160	160	298.15	3.965		
C	47.93102	180	280	303.15	3.971		
		200	550	303.15	4.034		
		220	1600	313.15	4.358		
		240	3400	313.15	4.520		
		260	6500	313.15	4.364		
		280	15000				

empirical eq.

ln x = A + B/τ + C ln τ

τ = (T/K)/298.15

A	–53.6887
B	39.4055
C	41.1210

FIGURE 2.1.1.2.11.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for ethylcyclohexane.

TABLE 2.1.1.2.11.2
Reported vapor pressures and Henry's law constants of ethylcyclohexane 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)		

Vapor pressure						Henry's law constant	
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Dohányosová et al. 2004	
Ebulliometry		Summary of literature data		Selected values		From solute fugacity *f* and *x*	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³ mol⁻¹)
51.412	6351	−14.5	133.3	20.6	1333	0	10422
55.636	7653	9.2	666.6	33.4	2666	5	14994
59.315	8959	20.6	1333	41.48	4000	10	20880
62.655	10299	33.4	2666	47.57	5333	15	28440
65.755	11691	47.6	5333	51.494	6666	20	37800
69.948	13818	56.7	7999	56.656	7999	25	48960
74.738	16615	69.0	13332	63.493	10666	30	62100
79.587	19916	87.8	26664	69.093	13332	35	77040
84.115	23451	109.1	53329	79.699	19998	40	93780
90.158	28956	131.8	101325	87.762	26664		
95.716	34893			94.327	33331		
102.412	43320	mp/°C	−111.3	99.906	39997		
109.327	53657			109.13	53329		
116.709	66760			116.666	66661		
124.723	83722			123.088	79993		
130.379	97609			128.715	93326		

(Continued)

TABLE 2.1.1.2.11.2 (*Continued*)

Vapor pressure						Henry's law constant	
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Dohányosová et al. 2004	
Ebulliometry		Summary of literature data		Selected values		From solute fugacity *f* and *x*	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³ mol⁻¹)
130.988	99208			129.764	95992		
131.551	100700			130.79	98659		
132.181	102404			131.795	101325		
132.742	103922			25.0	1707		
bp/°C	131.783			eq. 2	P/mmHg		
Antoine eq.				A	6.86728		
eq. 2	P/mmHg			B	1382.466		
A	6.87041			C	214.995		
B	1384.036			bp/°C	131.795		
C	214.128			ΔH_V/(kJ mol⁻¹) =			
temp range 51.4–132.7°C				at 25°C	40.48		
pressure range 48–780 mmHg				at bp	34.31		
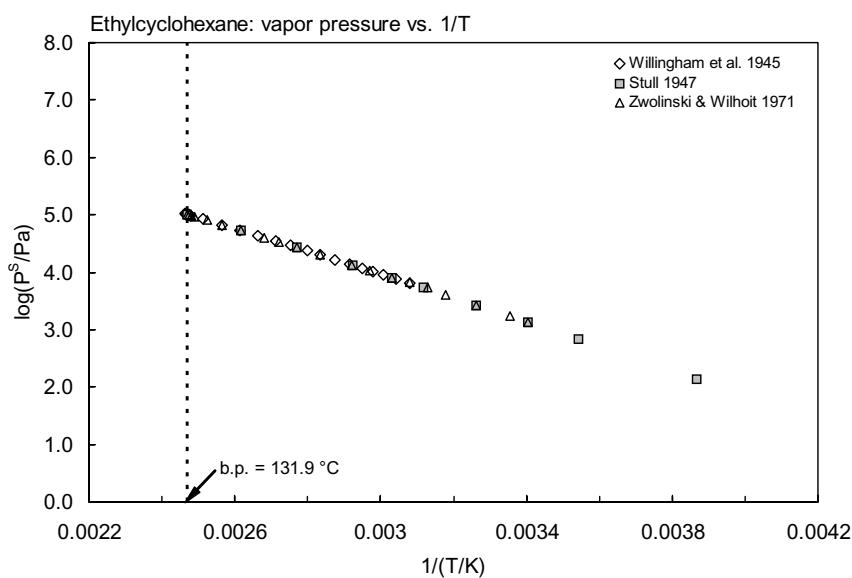
FIGURE 2.1.1.2.11.2 Logarithm of vapor pressure versus reciprocal temperature for ethylcyclohexane.
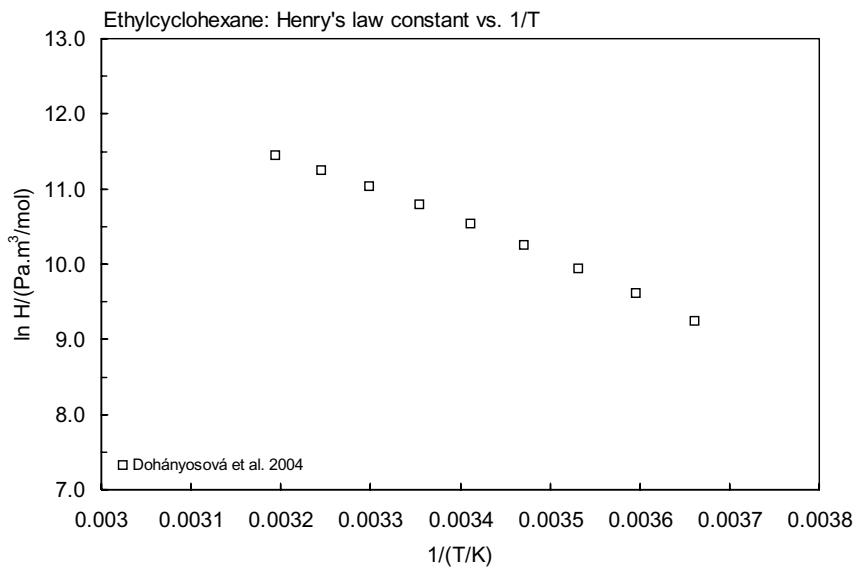
FIGURE 2.1.1.2.11.3 Logarithm of Henry's law constant versus reciprocal temperature for ethylcyclohexane.

2.1.1.2.12   Cycloheptane

Common Name: Cycloheptane
Synonym: suberane
Chemical Name: cycloheptane
CAS Registry No: 291-64-5
Molecular Formula: C_7H_{14}
Molecular Weight: 98.186
Melting Point (°C): –12
    –8.46   (Lide 2003)
Boiling Point (°C): 118.5
    118.4   (Lide 2003)
Density (g/cm³):
    0.8098   (20°C, Weast 1984)
    0.80656   (measured, Anand et al. 1975)
Molar Volume (cm³/mol):
    121.3   (20°C, calculated-density, Stephenson & Malanowski 1987)
    136.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    4.98, 0.29, 0.45, 1.88 (–138.35, –74.95, –60.75, –8.05°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    47.6, 48.2   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    30.0   (shake flask-GC, McAuliffe 1966)
    27.1   (30°C, shake flask-GC, Groves 1988)
    23.5, 23.5   (25, 30°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    19920*   (68.2°C, ebulliometry, measured range 68.2–159°C, Finke et al. 1956)
    log (P/mmHg) = 6.85271 – 1330.742/(t/°C + 216.246); temp range 68.2–159°C (Antoine eq., ebulliometry, Finke
        et al. 1956)
    2924*   (static method-quartz spiral gauge, measured range 283.048–323.551 K, Anand et al. 1975)
    log (P/kPa) = 6.19317 – 1450.17/(T/K – 44.91); temp range 283.048–323.551 K (static method, vapor-liquid
        equilibria study, Anand et al. 1975)
    16312*   (63.03°C, comparative ebulliometry, measured range 60–121.7°C, Meyer & Hotz 1976)
    log (P/mmHg) = 5.85683 – 1333.780/(t/°C + 216.6438); temp range 60–121.7°C (Antoine eq., comparative
        ebulliometry, Meyer & Hotz 1976)
    log (P/atm) = [1– 391.896/(T/K)] × 10^{0.885524 – 8.19621 × 10^{-4}·(T/K) + 7.88065 × 10^{-7}·(T/K)²}; temp range:
        284.35–432.17 K (Cox eq., Chao et al. 1983)
    2895, 2898 (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.97858 – 1331.383/(214.325 + t/°C); temp range 60.2–159°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    log (P/kPa) = 5.98198 – 1333.899/(216.657 + t/°C); temp range 63.03–121.68°C (Antoine eq. from reported
        exptl. data, Boublik et al. 1984)
    2895   (extrapolated-Antoine eq., Dean 1985, 1992)
    log (P/mmHg) = 6.85395 – 1331.57/(216.35 + t/°C); temp range: 68–159°C (Antoine eq., Dean 1985, 1992)
    2930   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.98143 - 1333.833/(-56.458 + T/K)$; temp range 341–433 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.12682 - 1417.738/(-47.665 + T/K)$; temp range 282–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.97596 - 1329.98/(-56.968 + T/K)$; temp range 333–398 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 7.05325 - 2475.271/(108.392 + T/K)$; temp range 476–604 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P/mmHg) = 54.0858 - 3.6109 \times 10^3/(T/K) - 17.331 \cdot \log (T/K) + 7.5292 \times 10^{-3} \cdot (T/K) + 1.7553 \times 10^{-6} \cdot (T/K)^2$; temp range 265–604 K (vapor pressure eq., Yaws 1994)

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

9977 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.87 (calculated-π substituent constant, Hansch et al. 1968)
3.06 (calculated-MCI χ, Murray et al. 1975)
3.76 (calculated-fragment const., Yalkowsky & Morozowich 1980)
2.72 (calculated-molar volume V_M, Wang et al. 1992)
3.91 (calculated-fragment const., Müller & Klein 1992)
3.1648 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.00 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{OH} = 13.1 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1985)
$k_{OH} = (7.88 \pm 1.38) \times 10^{12}$ cm³ mol⁻¹ s⁻¹ at 298 K (flash photolysis-resonance absorption, Jolly et al. 1985)
$k_{OH} = (11.8 - 13.1) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298–300 K (review, Atkinson 1989)
$k_{OH} = 1.25 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1990)
$k_{OH} = 13.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.12.1
Reported vapor pressures of cycloheptane 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)	
$\log P = A'[1 - (T_B/K)/(T/K)]$	(5) where $A' = a + bT + cT^2$	

Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976	
ebulliometric method		static-quartz spiral gauge		comparative ebulliometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
68.204	19920	283.043	1272	63.03	16312
74.338	25007	288.237	1711	68.929	20748
80.529	31160	292.906	2218	77.747	28258
86.771	38547	298.150	2924	85.702	37172
93.068	47359	301.924	3550	96.324	52481
99.416	57803	309.193	5080	106.462	71394
105.820	70109	312.723	6006	117.547	97871
112.281	84525	317.813	7573	121.681	109500
118.793	101325	323.551	9741		
125.364	120798			bp/°C	118.813
131.985	143268	Antoine eq.			
138.665	169052	eq. 3	P/kPa	Antoine eq.	
145.387	198530	A	6.19317	eq. 2	P/cmHg
152.178	232087	B	1450.17	A	5.85683
159.022	270110	C	–44.91	B	1333.780
				C	216.6438
bp/°C	118.79			temp range: 63–122°C	
$\Delta H_V =$	38.53 kJ/mol				
	at 25°C			Cox equation:	
Antoine eq.				eq 5	P/atm
eq. 2	P/mmHg			a	0.878453
A	6.85271			$-b \times 10^3$	0.916539
B	1330.742			$c \times 10^6$	0.965009
C	216.246				
Cox eq.					
eq. 5	P/atm				
T_B	391.953				
a	0.839608				
$-b \times 10^4$	6.9133				
$c \times 10^7$	6.4035				
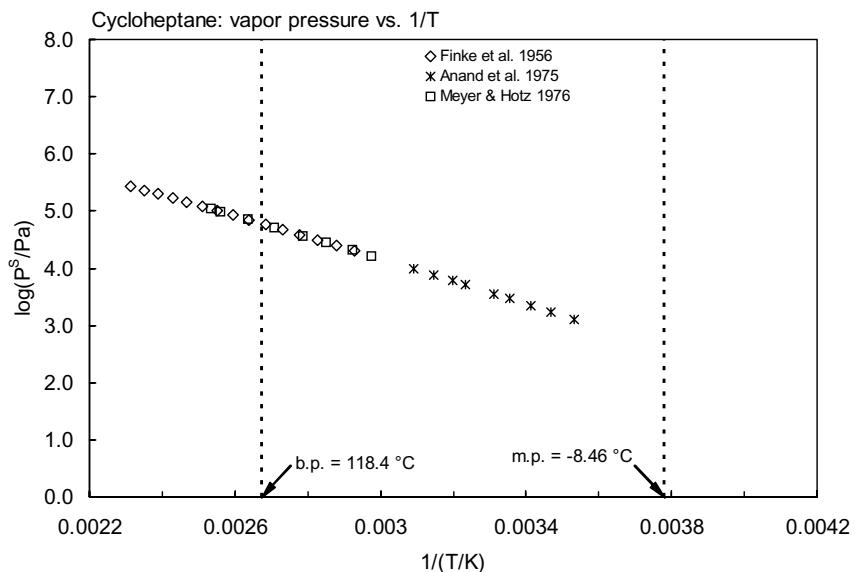
FIGURE 2.1.1.2.12.1 Logarithm of vapor pressure versus reciprocal temperature for cycloheptane.

2.1.1.2.13 Cyclooctane

Common Name: Cyclooctane
Synonym:
Chemical Name: cyclooctane
CAS Registry No: 292-64-8
Molecular Formula: C_8H_{16}
Molecular Weight: 112.213
Melting Point (°C):
    14.59   (Lide 2003)
Boiling Point (°C): 151
    149   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.8340   (Weast 1984)
Molar Volume (cm^3/mol):
    134.4   (20°C, calculated-density, Stephenson & Malanowski 1987)
    154.1   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.32, 0.48, 2.41 (−106.65, −89.35, 14.85°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    48.89, 51.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C and the reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    7.90   (shake flask-GC, McAuliffe 1966)
    7.48   (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)
    5.80*   (generator column-GC, measured range 27.15–313.15 K, Dohányosová et al. 2004)
    $\ln x = -55.1375 + 41.2528/\tau + 43.2804 \cdot \ln \tau$; $\tau = T/298.15$ K (empirical eq., generator column-GC, Dohányosová
        et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    19920*   (96.7°C, ebulliometry, measured range 96.7–194.4°C, Finke et al. 1956)
    log (P/mmHg) = 6.86173 − 1437.682/(t/°C + 210.003); temp range 96.7–194.4°C (Antoine eq., ebulliometry,
        Finke et al. 1956)
    748*   (static-quartz spiral gauge, measured range 290.961–323.326 K, Anand et al. 1975)
    log (P/kPa) = 5.97188 − 1447.45/(T/K − 60.67); temp range 291–323 K (static method, vapor-liquid equilibria
        VLE study, Anand et al. 1975)
    22454*   (100.133°C, comparative ebulliometry, measured range 100.1–161°C, Meyer & Hotz 1976)
    log (P/mmHg) = 5.861786 − 1438.455/(t/°C + 210.1844); temp range 100.1–161°C (Antoine eq., comparative
        ebulliometry, Meyer & Hotz 1976)
    767, 740   (extrapolated-Antoine eq., extrapolated, Boublik et al. 1984)
    log (P/kPa) = 5.98693 − 1437.751/(210.012 + t/°C); temp range 96.7–194.4°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    log (P/kPa) = 6.06524 − 1492.101/(216.413 + t/°C); temp range 100.1–160.9°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    740   (extrapolated-Antoine eq., Dean 1985, 1992)
    log (P/mmHg) = 6.86187 − 1437.79/(210.02 + t/°C); temp range 97–194°C (Antoine eq., Dean 1985, 1992)
    753   (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.98663 - 1437.682/(-63.147 + T/K)$; temp range 369–487 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.9899 - 1440.707/(-62.701 + T/K)$; temp range 369–468 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.20474 - 1564.985/(-50.842 + T/K)$; temp range 289–369 K (Antoine eq.-III, Stephenson & Malanowski 1987)

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

10485   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

14526*   (derived from solute fugacity and mole fraction solubility, temp range 273.15–313.15 K, Dohányo-sová et al. 2004)

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

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

3.50   (calculated-MCI χ, Murray et al. 1975)

3.28   (Hutchinson et al. 1980; Sangster 1989)

3.28   (calculated-fragment const., Lyman 1982)

4.45   (recommended, Sangster 1989)

3.04   (calculated-molar volume V$_M$, Wang et al. 1992)

4.47   (calculated-fragment const., Müller & Klein 1992)

3.6117   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:

Photolysis:

Oxidation: 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$_{OH}$ = 14.0 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric t$_{1/2}$ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.13.1
Reported aqueous solubilities and Henry's law constants of cyclooctane at various temperatures

Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC		smoothed exptl raw data		from solute fugacity f and x	
T/K	S/g·m⁻³	T/K	S/g·m⁻³	T/K	H/(Pa m³/mol)
	raw data				
274.15	5.53	273.15	5.73	273.15	2826
274.15	5.885	278.15	5.59	278.15	4158
278.15	5.548	283.15	5.53	283.15	5922
278.15	5.442	288.15	5.55	288.15	8190
283.15	5.548	293.15	5.64	293.15	11052
288.15	5.754	298.15	5.80	298.15	14526
293.15	5.492	303.15	6.02	303.15	18720
298.15	5.848	308.15	6.32	308.15	23400
298.15	5.530	313.15	6.68	313.15	28800
303.15	5.922				
303.15	5.835	ln x = A + B/τ + C ln τ			
308.15	6.483	τ = T/298.15			
308.15	6.421	A	–55.1375		
313.15	6.733	B	41.2528		
313.15	6.858	C	43.2804		
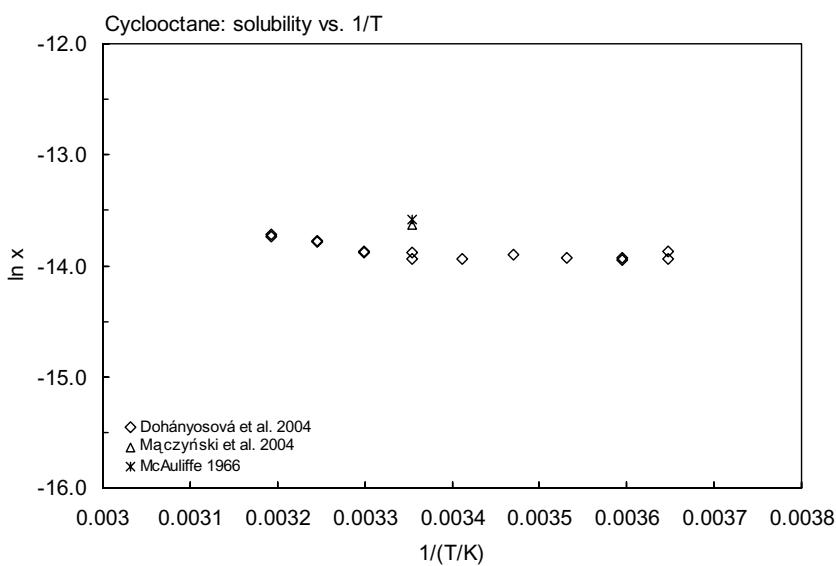
FIGURE 2.1.1.2.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclooctane.
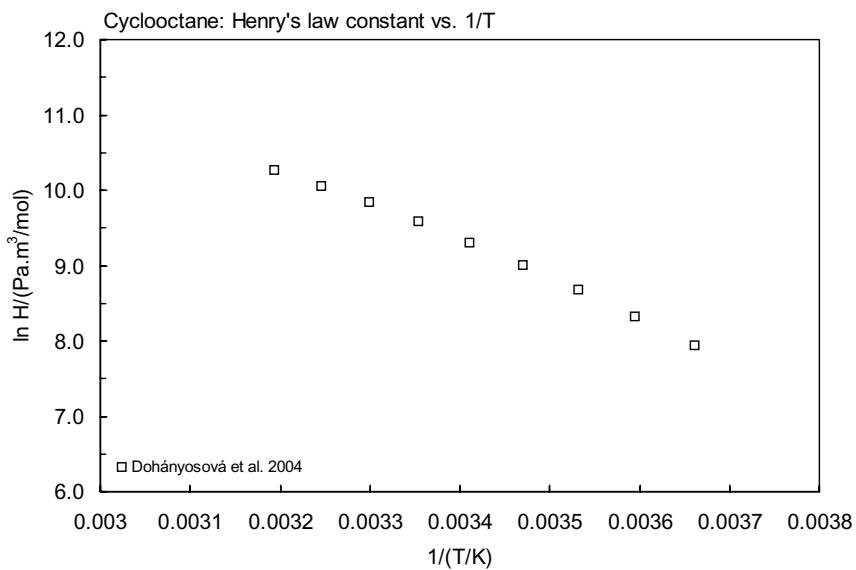
FIGURE 2.1.1.2.13.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctane.

TABLE 2.1.1.2.13.2

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

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

Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976		Dohányosová et al. 2004	
ebulliometry		static-quartz spiral gauge		comparative ebulliometry		from Anand et al. 1975	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa
96.711	19920	290.961	488	100.133	22454	273.15	207
103.318	25007	294.376	601	108.375	29598	278.15	292
109.977	31160	298.150	748	118.813	41155	283.15	406
116.694	38457	302.060	944	127.569	53410	288.15	557
123.472	47359	306.922	1244	139.435	74511	293.15	753
130.301	70109	311.678	1605	149.031	95919	303.15	1010
137.190	84525	316.472	2056	157.388	118293	308.15	1330
144.133	101325	323.326	2890	160.911	129263	313.15	1730
151.146	120798						
158.203	143268	Antoine eq.		bp/°C	151.148		
165.321	169052	eq. 3	P/kPa	Antoine eq.			
172.502	198530	A	6.91788	eq. 2	P/cmHg		
187.040	232087	B	1447.45	A	5.861786		
194.397	270110	C	−60.67	B	1438.455		
				C	210.1844		
bp/°C	151.14			temp range 100–161°C			
Antoine eq.							
eq. 2	P/mmHg			Cox equation:			

(Continued)

TABLE 2.1.1.2.13.2 (*Continued*)

Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976		Dohányosová et al. 2004	
ebulliometry		static-quartz spiral gauge		comparative ebulliometry		from Anand et al. 1975	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa
A	686173			eq 5	P/atm		
B	1437.682			a	0.869777		
C	210.003			$-b \times 10^3$	0.775348		
				$c \times 10^6$	0.716695		
Cox equation:							
eq 5	P/atm						
a	0.839609						
$-b \times 10^4$	6.2033						
$c \times 10^7$	5.177						
T_B	424.300						
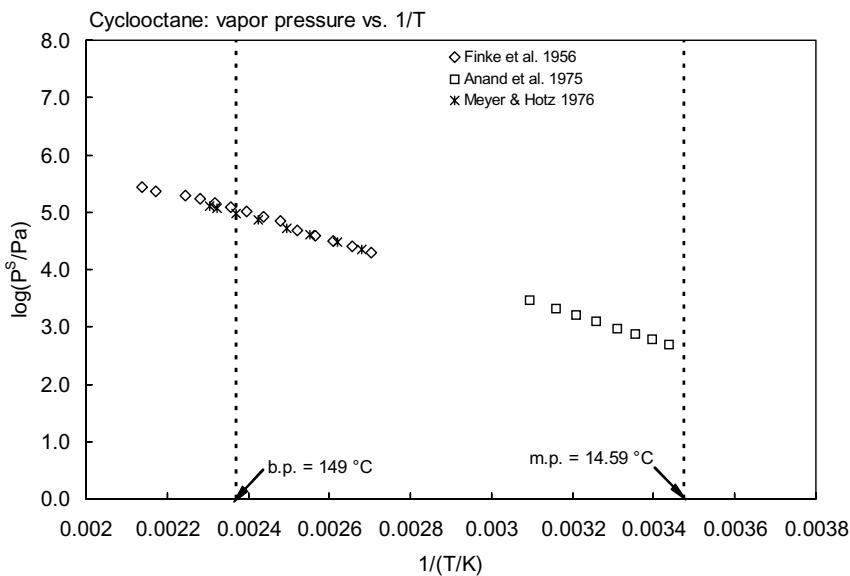
FIGURE 2.1.1.2.13.3 Logarithm of vapor pressure versus reciprocal temperature for cyclooctane.

2.1.1.2.14   Decalin
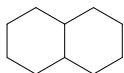
Common Name: Decalin
Synonym: bicyclo[4.4.0]decane, naphthalane, naphthane
Chemical Name: decahydronaphthalene (mixed isomers)
CAS Registry No: 91-17-8
Molecular Formula: $C_{10}H_{18}$
Molecular Weight: 138.250
Melting Point (°C):
    –42.9   (*cis*-decalin, Lide 2003)
    –30.4   (*trans*-decalin, Lide 2003)
Boiling Point (°C): 191.7
    195.774   (*cis*-decalin, Camin & Rossini 1955)
    187.273   (*trans*-decalin, Camin & Rossini 1955)
    191.7   (Riddick et al. 1986)
Density (g/cm³ at 20°C):
    0.8865, 0.8789   (20°C, 25°C, mixed isomers, Riddick et al. 1986)
Molar Volume (cm³/mol):
    154.8, 159.6 (*cis*-decalin, *trans*-decalin, calculated-density, Stephenson & Malanowski 1987)
    184.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.09   (bp, mixed isomers, Riddick et al. 1986)
    51.342, 40.999   (*cis*-decalin, 25°C, bp, Riddick et al. 1986)
    49.87, 40.229   (*trans*-decalin, 25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    14.414, 9.489   (*cis*-decalin, *trans*-decalin, Riddick et al. 1986)
    14.43   (*cis*-decalin, Chickos et al. 1999)
    2,13, 9.49   (*trans*-decalin, –57.05, 42.95°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    59.45, 52.1 (*cis*-decalin: exptl., calculated-group additivity method, Chickos et al. 1999)
    51.1, 52.1 (*trans*-decalin: exptl, calculated-group additivity method, total phase change entropy, Chickos et al.
            1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.889   (shake flask-GC, Price 1976; quoted as more reliable value, Shaw 1989)
    6.21   (shake flask-GC, Hutchinson et al. 1980)
    1.99   (calculated-QSAR, Passino & Smith 1987)
    2.14   (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

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*   (23.3°C, isomer not specified, ebulliometry, measured range 23.3–150.0°C, Gardner & Brewer 1937)
    241*   (20°C, *cis*-decalin, manometry, measured range –29.5 to 194.7°C, Seyer & Mann 1945)
    381*   (13°C, *trans*-decalin, manometry, measured range –30.0 to 235.3°C, Seyer & Mann 1945)
    133.3*   (22.5°C, *cis*-decalin, summary of literature data, temp range 22.5–194.6°C, Stull 1947)
    666.6*   (30.6°C, *trans*-decalin, summary of literature data, temp range –0.80 to 186.7°C, Stull 1947)
    5529*   (99.883°C, *cis*-decalin, ebulliometry, measured range 99.883–196.376°C, Camin & Rossini 1955)
    5530*   (92.36°C, *trans*-decalin, ebulliometry, measured range 92.36–187.867°C, Camin & Rossini 1955)

log (P/mmHg) = 6.87529 – 1594.460/(203.392 + t/°C); temp range 99.8–196.4°C (*cis*-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)

log (P/mmHg) = 6.85681 – 1564.683/(206.259 + t/°C); temp range 92.3–187.0°C (*trans*-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)

104*, 164* (*cis*-decalin, *trans*-decalin, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.87529 – 1594.460/(203.392 + t/°C); temp range 68.0–277.67°C (*cis*-decalin, Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.85681 – 1564.683/(206.259 + t/°C); temp range 60.91–218.88°C (*trans*-decalin, Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 10515.4/(T/K)] + 7.797540; temp range 22.5–194.6°C (*cis*-decalin, Antoine eq., Weast 1972–73)

log (P/mmHg) = [–0.2185 × 8749.1/(T/K)] + 6.973042; temp range –0.80 to 186.7°C (*trans*-decalin, Antoine eq., Weast 1972–73)

log (P/atm) = [1– 468.915/(T/K)] × 10^{0.683577 – 0.900942 × 10^{-4}·(T/K) + 2.28255 × 10^{-7}·(T/K)^2}; temp range 295.65–727.59 K (*cis*-decalin, Cox eq., Chao et al. 1983)

log (P/atm) = [1– 460.458/(T/K)] × 10^{0.880979 – 6.38749 × 10^{-4}·(T/K) + 4.59180 × 10^{-7}·(T/K)^2}; temp range: 365.51–461.02 K, (*trans*-decalin, Cox eq., Chao et al. 1983)

178, 104 (*cis*-decalin, calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.96043 – 2358.398/(280.79 + t/°C); temp range –29.5 to 194.7°C (*cis*-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.00042 – 1594.653/(203.415 + t/°C); temp range 99.88–196.4°C (*cis*-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

434, 165 (*trans*-decalin, calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 7.69594 – 3126.688/(363.012 + t/°C); temp range –30.0 to 253.3°C (*trans*-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.98704 – 1568.642/(206.726 + t/°C); temp range 92.36–187.9°C (*trans*-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

104, 168 (*cis*-, *trans*-decalin, Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.87529 – 1594.81/(203.39 + t/°C), temp range 68–228°C (*cis*-decalin Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.86581 – 1564.683/(206.26 + t/°C); temp range 61–219°C (*trans*-decalin Antoine eq., Dean 1985, 1992)

130 (mixed isomer, 23.3°C, lit. average, Riddick et al. 1986)

100, 164 (selected lit., *cis*-, *trans*-decalin, Riddick et al. 1986)

log (P/kPa) = 6.00019 – 1594.460/(203.392 + t/°C), temp range not specified (*cis*-decalin, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.98171 – 1564.683/(206.259 + t/°C), temp range not specified (*trans*-decalin, Antoine eq., Riddick et al. 1986)

105, 168 (*cis*-decalin, *trans*-decalin, extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.00019 – 1595.176/(–69.622 + T/K); temp range 371–473 K (*cis*-decalin, Antoine eq., Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 5.99363 – 1573.981/(–65.77 + T/K); temp range 363–461 K (*trans*-decalin, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 45.6345 – 4.21 × 10^3/(T/K) – 12.881·log (T/K) – 7.8083 × 10^{-11}·(T/K) + 2.8637 × 10^{-6}·(T/K)^2; temp range 230–702 K (*cis*-decalin, vapor pressure eq., Yaws 1994)

log (P/mmHg) = 76.1002 – 5.03 × 10^3/(T/K) – 25.078·log (T/K) + 9.7608 × 10^{-3}·(T/K) – 2.5814 × 10^{-6}·(T/K)^2; temp range 243–687 K (*trans*-decalin, vapor pressure eq., Yaws 1994)

128* (20.42°C, *trans*-decalin, differential pressure gauge, measured range –29.31 to 160.7°C, Mokbel et al. 1995)

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.):

11855* (EPICS-GC/FID, measured range 10–30°C Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 11.85 – 4125/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

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

    4.79   (calculated-fragment const., Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

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

        $k_{OH} = 1.96 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} of *cis*-decalin and 2.02×10^{-11} cm^3 molecule^{-1} s^{-1} of *trans*-decalin at
           299 K (Atkinson 1985)

        $k_{OH} = 2.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction at 298 K (Atkinson 1990)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

TABLE 2.1.1.2.14.1

Reported vapor pressures and Henry's law constants of decalin (isomer not specified) 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)			

Vapor pressure				Henry's law constant	
Gardner & Brewer 1937				Ashworth et al. 1988	
ebulliometry				EPICS-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
23.3	133.3	60.0	987	10	7093
32.8	240	66.1	1293	15	8481
37.3	280	86.8	3520	20	10740
38.4	320	96.0	5186	25	11855
42.5	400	104.5	7293	30	20164
43.0	413	118.8	11652		
49.6	587	133.8	20278	ln H = A – B/(T/K)	
50.6	627	150.0	31997	eq. 4a	H/(atm m³/mol)
54.3	747			A	11.85
54.6	800	bp/°C	193.8	B	4125
59.8	1027				
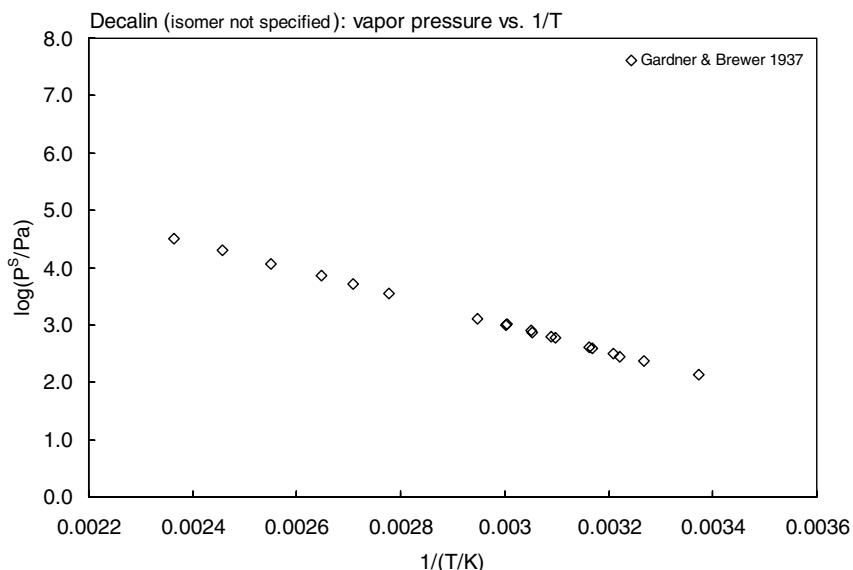
FIGURE 2.1.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for decalin.
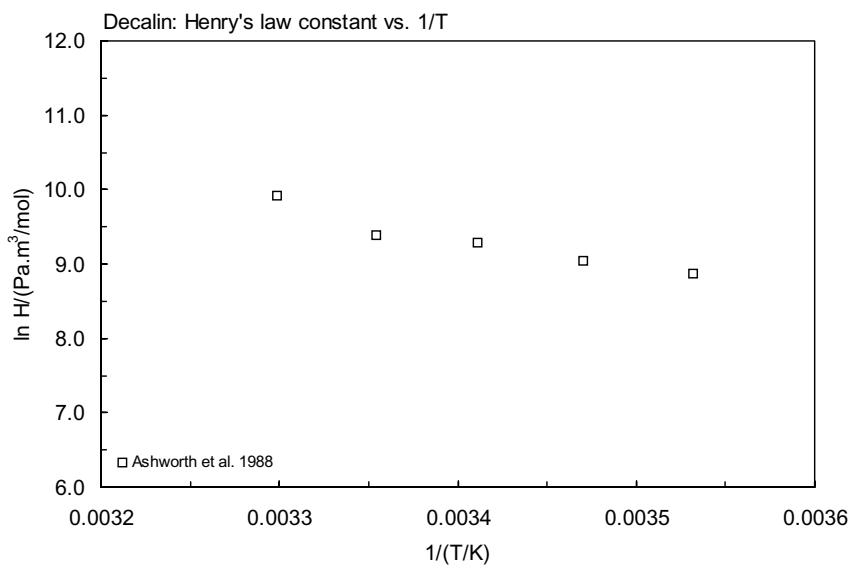
FIGURE 2.1.1.2.14.2 Logarithm of Henry's law constant versus reciprocal temperature for decalin.

TABLE 2.1.1.2.14.2
Reported vapor pressures of *cis*-decalin 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)	$\ln P = A - B/(T/K) - C·\ln (T/K)$ (4a)

Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–29.5	51	22.5	133.3	99.883	5529	68.0	1333
–19.2	87	50.1	666.6	105.685	6941	82.64	2666
–10.0	115	64.2	1333	110.490	8331	91.97	4000
0.0	145	79.8	2666	114.152	9523	98.998	5333
12.0	196	97.2	5333	118.004	10943	104.609	6666
20.0	241	108.0	7999	123.132	13008	109.391	7999
38.0	457	123.2	3332	128.731	15827	117.280	10666
43.4	532	145.4	26664	135.021	19433	123.676	13332
49.9	704	169.9	53329	140.176	22881	135.934	19998
50.4	719	194.6	101325	147.456	28546	145.171	26664
52.9	805			154.245	34817	152.718	33331
56.9	971	mp/°C	–43.3	161.885	43164	159.127	39997
10.0	1095			170.056	53773	169.767	53329
70.0	1669			178.629	67068	178.349	66661
80.1	2590			187.823	83031	185.724	79993
92.4	4358			194.370	98080	192.251	93326
105.1	7239			195.055	99658	193.389	95992
109.8	8389			195.635	101001	194.622	98659
112.4	9121			196.376	102727	195.774	101325
124.6	13976						
148.7	29997			bp/°C	195.774		
172.7	57690			eq. 2	P/mmHg	eq. 2	P/mmHg
194.700	101093			A	6.87529	A	6.87529
				B	1594.460	B	1594.460
eq. 4a	P/cmHg			C	203.392	C	203.392
A	6.8139					bp/°C	195.774
B	1702.20					$\Delta H_v/(kJ\ mol^{-1}) = 39.30$	
C	34.32						at bp
bp/°C	194.5						
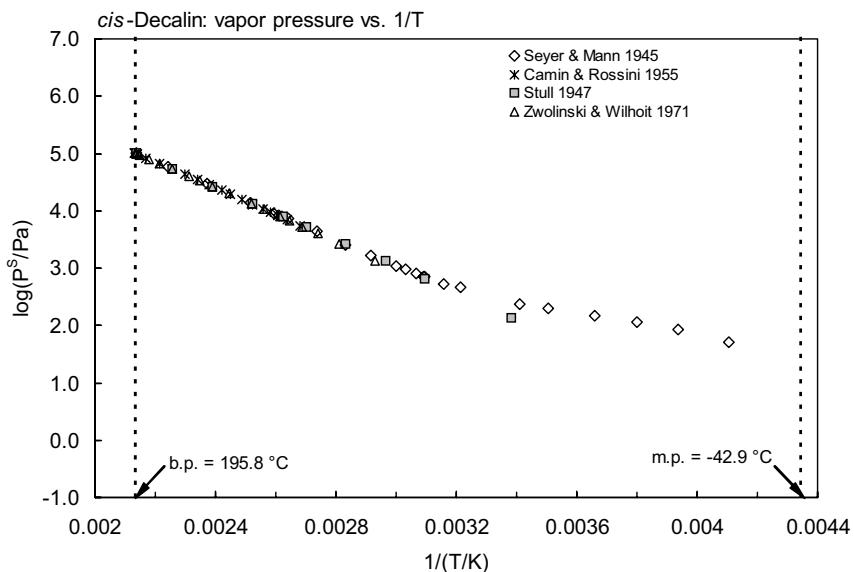
FIGURE 2.1.1.2.14.3 Logarithm of vapor pressure versus reciprocal temperature for *cis*-decalin.

TABLE 2.1.1.2.14.3
Reported vapor pressures of *trans*-decalin 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)	ln P = A – B/(T/K) – C·ln (T/K)	(4a)

1.

Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–30.0	59	–0.80	133.3	92.36	5530	60.91	1333
–24.1	80	30.6	666.6	98.129	6942	75.37	2666
–11.1	143	47.2	1333	102.891	8331	84.59	4000
–0.70	229	65.3	2666	106.500	9522	91.527	5333
0.0	241	85.7	5333	110.316	10946	97.072	6666
13.0	381	98.4	7999	115.356	13086	101.800	7999
30.9	801	114.6	13332	120.918	15828	109.599	10666
51.5	1597	136.2	26664	127.140	19434	115.922	13332
59.7	2221	160.1	53329	132.255	22434	128.045	19998
65.3	2657	186.7	101325	146.156	34817	137.182	26664
74.4	3562			153.719	43163	144.649	33331
83.5	5072	mp/°C	–30.7	161.801	53773	150.991	39997
95.5	7307			170.297	67069	161.522	53329
112.4	12635			179.395	84031	170.018	66661
119.4	16087			185.885	98081	177.320	79993
136.7	27478			186.563	99665	183.783	93326
152.3	42595			187.140	101005	184.911	95992
168.0	65024			187.867	102731	186.132	98659

TABLE 2.1.1.2.14.3 *(Continued)*

Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
187.1	103009					187.274	101325
209.8	170060			bp/°C	187.273		
212.9	185496						
223.4	228787			eq. 2	P/mmHg	eq. 2	P/mmHg
235.3	284978			A	6.85681	A	6.83561
				B	1564.683	B	1564.683
bp/°C	185.8			C	206.259	C	206.269
eq. 4a	P/cmHg					bp/°C	187.274
A	6.8509					$\Delta H_v/(kJ\ mol^{-1}) = 38.50$	
B	2182.38						at bp
C	32.64						

2.

		Mokbel et al. 1995					
		static method-manometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
−29.31	1.91	40.37	448	99.60	7347		
−19.37	5.23	50.42	790	109.58	10670		
−9.42	13.2	60.41	1329	119.69	15160		
0.46	29.4	64.63	1636				
10.44	63.1	69.55	2050	data fitted to Wagner eq.			
20.42	128	79.48	3219				
30.35	245	89.54	4939				
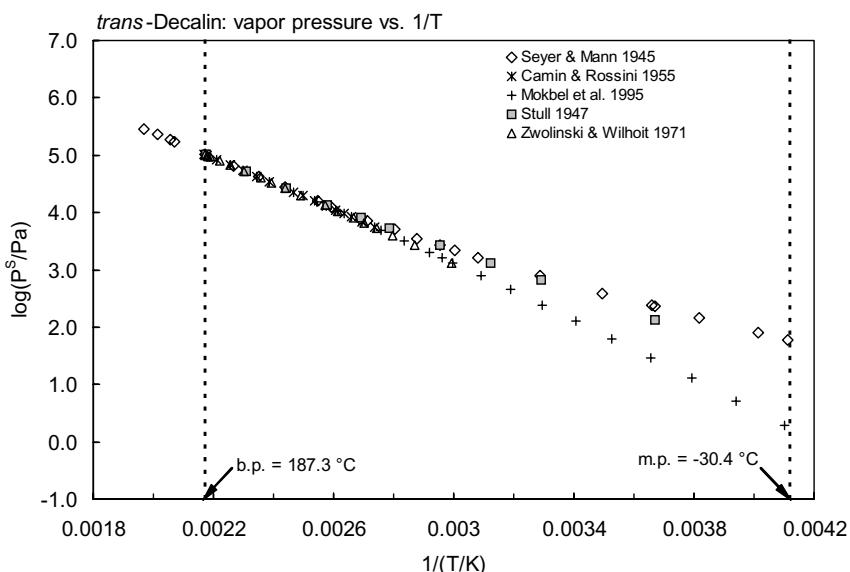
FIGURE 2.1.1.2.14.4 Logarithm of vapor pressure versus reciprocal temperature for *trans*-decalin.

2.1.2 UNSATURATED HYDROCARBONS

2.1.2.1 Alkenes

2.1.2.1.1 2-Methylpropene

Common Name: 2-Methylpropene
Synonym: isobutene, isobutylene
Chemical Name: 2-methylpropene
CAS Registry No: 115-11-7
Molecular Formula: C_4H_8; $CH_3C(CH_3)CH_2$
Molecular Weight: 56.107
Melting Point (°C):
　　–140.7　　　(Lide 2003)
Boiling Point (°C):
　　–6.9　　　(Dreisbach 1959; Lide 2003)
Density (g/cm³ at 20°C):
　　0.5942, 0.5879　　　(20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
　　94.4　　　(20°C, calculated-density, McAuliffe 1966)
　　95.4　　　(25°C, calculated-density)
　　88.8　　　(calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
　　5.92　　　(Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
　　44.72, 41.8　(exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
　　263　　　　　(shake flask-GC, of liquid at 1 atmospheric pressure, McAuliffe 1966)

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.):
　　131695*, 131855　　(0°C, static method-manometer, measured range –56.75 to 0°C, Lamb & Roper 1940)
　　101325*　　　　　(–6.9°C, summary of literature data, temp range –105.1 to –6.9°C, Stull 1947)
　　303700　　　　　(calculated from determined data, Dreisbach 1959)
　　log (P/mmHg) = 6.84134 – 923.2/(240.0 + t/°C); temp range –68 to 39°C (Antoine eq. for liquid state, Dreisbach 1959)
　　302642*　　　　　(extrapolated-Antoine eq., temp range –81.95 to 11.88°C, Zwolinski & Wilhoit 1971)
　　log (P/mmHg) = 6.84134 – 923.200/(240.00 + t/°C); temp range –81.95 to 11.88°C (Antoine eq., Zwolinski & Wilhoit 1971)
　　log (P/mmHg) = [–0.2185 × 5742.9/(T/K)] + 7.601563; temp range –105.1 to –6.90°C (Antoine eq., Weast 1972–73)
　　log (P/mmHg) = 6.68466 – 886.25/(234.64 + t/°C); temp range –82 to 12°C (Antoine eq., Dean 1985, 1992)
　　303255　　　　　(interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
　　log (P_L/kPa) = 5.96624 – 923.2/(–33.15 + T/K); temp range 212–279 K (Antoine eq.-I, Stephenson & Malanowski 1987)
　　log (P_L/kPa) = 5.93211 – 907.644/(–35.082 + T/K); temp range 266–313 K (Antoine eq.-II, Stephenson & Malanowski 1987)
　　log (P_L/kPa) = 6.27428 – 1095.288/(–9.441 + T/K); temp range 310–376 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 7.64267 – 2336.466/(160.311 + T/K)$; temp range 371–418 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log $(P/mmHg) = 39.2295 – 2.1094 \times 10^3/(T/K) – 12.567 \cdot log (T/K) + 7.7304 \times 10^{-3} \cdot (T/K) – 1.3659 \times 10^{-6} \cdot (T/K)^2$; temp range 133–418 K (vapor pressure eq., Yaws 1994)

607940   (45.44°C, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)

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

21600   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

23100, 10800   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

14800   (calculated-P/C, Mackay & Shiu 1981)

35800   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

20994   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

0.64, 1.32   (quoted, calculated-molar volume V_M, Wang et al. 1992)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O3} = 6.2 \times 10^{-18}$ cm³ molecule^{-1} s^{-1} at room temp. (Hanst et al. 1958)

$k_{O3} = 2.32 \times 10^{-17}$ cm³ molecule^{-1} s^{-1} at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{OH} = 6.46 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{O3} = 13.6 \times 10^{-18}$ cm³ molecule$^{-1} \cdot$s^{-1} at room temp (Japar et al. 1974)

$k_{O3} = 11.7 \times 10^{-18}$ cm³ molecule^{-1} s^{-1} (Huie & Herron 1975)

$k_{OH} = (3.05 \pm 0.31) \times 10^{10}$ cm³ M^{-1} s^{-1} at 305 ± 2 K (relative rate method, Winer et al. 1976)

$k_{O(3P)} = 1.60 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} for the reaction with O(^{3}P) atoms (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)

$k_{OH}^* = 5.07 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 297.2 K, measured range 297–425 K (flash photolysis-resonance fluorescence, Atkinson & Pitts 1977)

$k_{O3} = 11.7 \times 10^{-18}$ cm³ molecule^{-1} s^{-1} at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)

$k_{OH} = 5.13 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = (6.46 \pm 0.13) \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Ohta 1984)

$k_{O3} = 5.14 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 5.14 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}; $k_{O3} = 1.21 \times 10^{-17}$ cm³ molecule^{-1} s^{-1} (review, Atkinson 1990)

$k_{OH} = 5.14 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}, $k_{NO3} = 31.3 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

$k_{NO3} = (3.15 – 3.38) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

$k_{OH}^* = 5.14 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}, $k_{NO3} = 3.32 \times 10^{-13}$ cm³ molecule^{-1} s^{-1}, $k_{O3}^* = 11.3 \times 10^{-18}$ cm³ molecule^{-1} s^{-1} and $k_{O(3P)} = 1.69 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 5.3 h, based on photooxidation rate constant k = 5.14×10^{-11} cm³·molecule^{-1} s^{-1} with OH radicals in air during summer daylight (Altshuller 1991).

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins and $t_{1/2} = 8.0$ d for substituted olefins, based on rate constant $k = 1 \times 10^6$ M^{-1} s^{-1} for oxidation by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.1.1
Reported vapor pressures of 2-methylpropene (isobutene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)	$\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2)	$\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)	
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)	
$\log P = A - B/(T/K) - C \cdot (T/K)$ (5)	

Lamb & Roper 1940		Stull 1947		Zwolinski & Wilhoit 1971			
static method-manometer		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–56.75	8725	–105.1	133.3	–81.95	1333	–8.983	93326
–25.30	47703	–96.5	666.6	–73.37	2666	–8.274	95992
–20.88	57462	–81.9	1333	–67.90	4000	–7.580	98659
–7.47	99791	–73.4	2666	–63.79	5333	–6.900	101325
–0.67	128789	–63.8	5333	–60.472	6666	25.0	302642
0.0	131695	–57.7	7999	–57.664	7999		
0.0	131855	–49.3	13332	–53.051	10666		
		–36.7	26664	–49.309	13332	eq. 2	P/mmHg
bp/°C	–7.12	–22.2	53329	–42.111	19998	A	6.84134
eq. 5	P/mmHg	–6.9	101325	–36.666	26664	B	923.200
A	9.77465			–32.231	33331	C	240.000
B	1503.866	mp/°C	–140.3	–28.462	39997	bp/°C	–6.90
C	0.0046649			–22.227	53329	$\Delta H_V/(kJ\ mol^{-1}) =$	
				–17.133	66661	at 25°C	20.59
				–12.789	79993	at bp	22.12
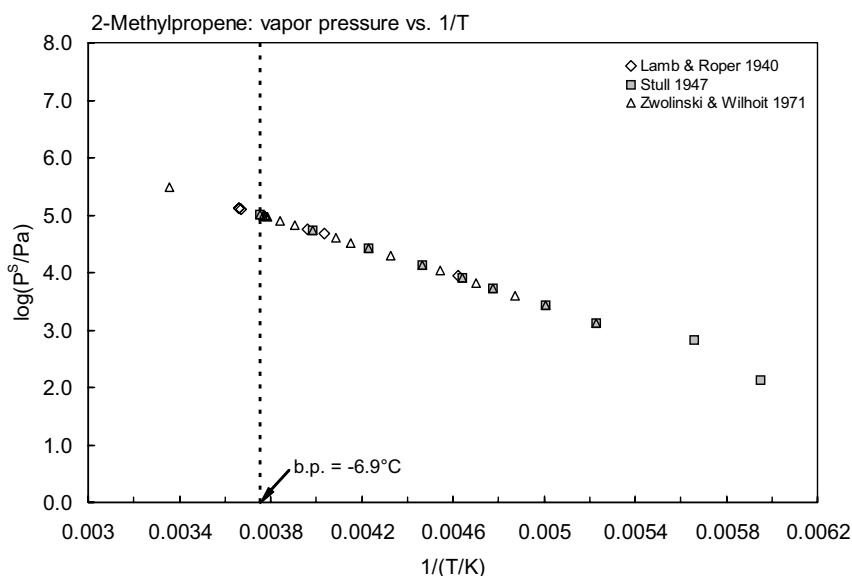
FIGURE 2.1.2.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpropene.

2.1.2.1.2   1-Butene

Common Name: 1-Butene
Synonym: butylene
Chemical Name: 1-butene
CAS Registry No: 106-98-9
Molecular Formula: C_4H_8; $CH_3CH_2CHCH_2$
Molecular Weight: 56.107
Melting Point (°C):
   –185.34 (Lide 2003)
Boiling Point (°C):
   –6.26   (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
   0.5951, 0.5888 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
   94.3   (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)
   95.3   (25°C, calculated-density)
   88.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   3.85   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   43.84, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

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

   222   (shake flask-GC, liquid at 1 atmospheric pressure, McAuliffe 1966)

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.):
   128536*   (0°C, static method-manometer, measured range –56.75 to 0°C, Lamb & Roper 1940)
   $\log (P/mmHg) = -1330.977/(T/K) – 0.0017607 \cdot (T/K) + 8.33816$; temp range 195–274 K (static method, Lamb & Roper 1940)
   361100*   (Antoine eq. regression, temp range –104.8 to –6.3°C, Stull 1947)
   296000   (calculated-Antoine eq., Dreisbach 1959)
   $\log (P/mmHg) = 6.84290 – 926.1/(240.0 + t/°C)$; temp range –67 to 40°C (Antoine eq. for liquid state, Dreisbach 1959)
   297309*   (derived from compiled data, Zwolinski & Wilhoit 1971)
   $\log (P/mmHg) = 6.84290 – 926.10/(240.00 + t/°C)$; temp range –81.5 to 12.6°C (Antoine eq., Zwolinski & Wilhoit 1971)
   $\log (P/mmHg) = [–0.2185 \times 5996.7/(T/K)] + 7.826754$; temp range –104.8 to –6.3°C (Antoine eq., Weast 1972–73)
   $\log (P/mmHg) = 6.531 – 810.261/(228.066 + t/°C)$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   $\log (P/mmHg) = 6.79290 – 908.80/(238.54 + t/°C)$; temp range –82 to 13°C (Antoine eq., Dean 1985, 1992)
   297020, 295800 (interpolated-Antoine eq.-III, V, Stephenson & Malanowski 1987)
   $\log (P_L/kPa) = 5.9678 – 926.1/(–33.15 + T/K)$; temp range 200–274 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   $\log (P_L/kPa) = 8.1706 – 1601.52/(7.059 + T/K)$; temp range 126–192 K (Antoine eq.-II, Stephenson & Malanowski 1987)
   $\log (P_L/kPa) = 6.05416 – 970.771/(–27.089 + T/K)$; temp range 267–345 K (Antoine eq.-III, Stephenson & Malanowski 1987)
   $\log (P_L/kPa) = 6.77294 – 1482/801/(48.073 + T/K)$; temp range 342–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
   $\log (P_L/kPa) = 6.27411 – 1097.171/(–9.657 + T/K)$; temp range 267–411 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/mmHg) = 27.3116 −1.9235 × 10^3/(T/K) −70.2064·log (T/K) + 7.4852 × 10^{-12}·(T/K) + 3.6481 × 10^{-6}·(T/K)^2; temp range 88–420 K (vapor pressure eq., Yaws 1994)

596140　　　　(50.12°C, vapor-liquid equilibrium VLE data, Pasanen et al., 2004)

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

25610　　　　　　　(calculated-P/C, Mackay & Shiu 1981)
25370　　　　　　　(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
26560, 15280　　　　(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
29800　　　　　　　(calculated-MCI χ, Nirmalakhandan & Speece 1988)
24800　　　　　　　(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.40; 2.17, 2.26, 2.43 (quoted; calculated-f const., Rekker 1977)
1.59, 1.32 (quoted, calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

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

k_{O3} = 1.03 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 30°C (flow system, Bufalini & Altshuller 1965)
k_{OH} = 4.08 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (discharge flow system-MS, Morris & Niki 1971)
k_{O3} = 1.23 × 10^{-17} cm^3 molecule^{-1} s^{-1} at room temp (Japar et al. 1974)
k_{O3} = 1.03 × 10^{-17} cm^3 molecule^{-1} s^{-1} at room temp (Huie & Herron 1975)
k_{OH} = (2.94, 2.96) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)
k_{O3} = 1.26 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 294 ± 2 K (static system-chemiluminescence, Adeniji et al. 1981)
$k_{O(3P)}$ = 4.20 × 10^{-12} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)
k_{OH}* = 3.53 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 297.2 K, measured range 297–425 K (flash photolysis-resonance fluorescence, Atkinson & Pitts, Jr. 1977)
k_{OH} = 3.13 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)
k_{OH} = 3.14 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH} = 3.14 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 1.10 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)
k_{OH} = 3.14 × 10^{-11} cm^3·molecule^{-1} s^{-1}, k_{NO3} = 1.23 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)
k_{OH} = 3.14 × 10^{-11} cm^3 molecule^{-1} s^{-1} with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)
k_{OH}* = 3.14 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{NO3}* = 1.35 × 10^{-14} cm^3 molecule^{-1} s^{-1}, and k_{O3}* = 9.64 × 10^{-18} cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)}$ = 4.15 × 10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 5.5 h, based on the reaction rate constant k = 3.14 × 10^{-11} cm^3 molecule^{-1} s^{-1} with OH radicals during summer daylight in the gas phase (Altshuller 1991).

Surface water: $t_{1/2}$ = 320 h and 9 × 10⁴ d for reaction with OH and RO$_2$ radicals of olefins in aquatic system, and $t_{1/2}$ = 7.3 d, based on oxidation reaction rate constant k = 3 × 10³ M⁻¹ s⁻¹ with singlet O$_2$ for unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.2.1
Reported vapor pressures of 1-butene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \qquad (1)$$
$$\log P = A - B/(C + t/°C) \qquad (2)$$
$$\log P = A - B/(C + T/K) \qquad (3)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K) \qquad (4)$$
$$\log P = A - B/(T/K) - C \cdot (T/K) \qquad (5)$$

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

| Lamb & Roper 1940		Stull 1947		Zwolinski & Wilhoit 1971			
static method-manometer		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–56.75	8549	–104.8	133.3	–81.5	1333	–8.35	93326
–25.3	45423	–89.4	666.6	–72.89	2666	–7.64	95992
–22.91	50436	–81.6	1333	–67.41	4000	–6.94	98659
–10.60	85513	–73.0	2666	–63.29	5333	–6.26	101325
–7.47	96992	–63.4	5333	–59.96	6666	25.0	297309
–0.67	125549	–57.2	7999	–57.15	7999		
0.0	128536	–48.9	13332	–52.52	10666	eq. 2	P/mmHg
		–36.2	26664	–48.77	13332	A	6.84290
bp/°C	–6.30	–21.7	53329	–41.56	19998	B	926.10
eq. 5	P/mmHg	–6.3	101325	–36.10	26664	C	240.00
A	6.33816			–31.65	33331	bp/°C	–6.26
B	1330.977	mp/°C	–130	–27.87	39997		
C	0.0017607			–21.62	53329	ΔH$_V$/(kJ mol⁻¹) =	
				–16.52	66661	at 25°C	20.13
				–12.16	79993	at bp	21.92
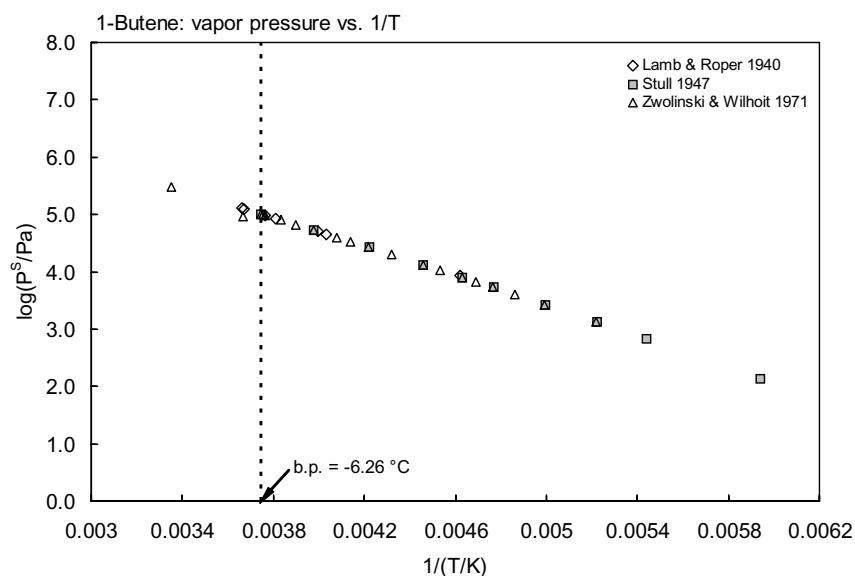
FIGURE 2.1.2.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butene.

2.1.2.1.3   2-Methyl-1-butene

Common Name: 2-Methyl-1-butene
Synonym:
Chemical Name: 2-methyl-1-butene
CAS Registry No: 563-46-2
Molecular Formula: C_5H_{10}, $CH_3CH_2C(CH_3)=CH_2$
Molecular Weight: 70.133
Melting Point (°C):
    –137.53   (Lide 2003)
Boiling Point (°C):
    31.2   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6504, 0.6451   (20°C, 25°C, at saturation pressure, Dreisbach 1959; Dean 1985)
Molar Volume (cm³/mol):
    107.8, 108.7   (20°C, 25°C, calculated-density)
    111.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.91   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    58.34, 48.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section.):
    215*   (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
    155   (estimated-nomograph of Kabadi & Danner 1979; Brookman et al. 1985)
    130   (misquoted from 3-methyl-1-butene, Wakita et al. 1986)
    168   (calculated-fragment solubility constants, Wakita et al. 1986)
    260   (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
    137   (calculated-molar volume V_M, Wang et al. 1992)
    128, 198   (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

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.):
    135540*   (interpolated-Antoine eq. regression, temp range –89.1 to 20.2°C, Stull 1947)
    70242*   (20.996°C, ebulliometry, measured range 1.155–62.675°C, Scott et al. 1949)
    log (P/mmHg) = 6.87314 – 1053.780/(232.768 + t/°C); temp range 1.155 to 62.675°C (Antoine eq., ebulliometry,
        Scott et al. 1949)
    81320   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.87314 – 1053.8/(233.0 + t/°C); temp range –38 to 75°C (Antoine eq. for liquid state, Dreisbach
        1959)
    81327*, 81330   (derived from compiled data, interpolated-Antoine eq., temp range –53.4 to 52.24°C Zwo-
        linski & Wilhoit 1971)
    log (P/mmHg) = 6.87314 – 1053.780/(232.788 + t/°C); temp range –53.4 to 52.24°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 6474.6/(T/K)] + 7.751419; temp range –89.1 to 20.2°C (Antoine eq., Weast 1972–73)
    82830   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.98834 – 1046.771/(232.181 + t/°C) temp range 1.115–63.68°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    99500   (interpolated-Antoine eq., temp range –53 to 52°C, Dean 1985, 1992)
    log (P/mmHg) = 6.84637 – 1039.69/(236.65 + t/°C); temp range –53 to 52°C (Antoine eq., Dean 1985, 1992)
    81360   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.99292 - 1050.937/(-40.727 + T/K)$; temp range 240–336 K (Antoine eq., Stephenson & Malanowski 1987)

log $(P/mmHg) = 30.2418 - 2.2723 \times 10^3/(T/K) - 8.1482 \cdot \log (T/K) + 5.2331 \times 10^{-11} \cdot (T/K) + 3.6802 \times 10^{-6} \cdot (T/K)^2$; temp range 136–465 K (vapor pressure eq., Yaws 1994)

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

43080   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

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

2.07   (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
1.89   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{OH} = 9.01 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{OH} = (6.37 \pm 0.16) \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Ohta 1984)

$k_{OH} = 9.01 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ to 6.07×10^{-11} cm³ molecule⁻¹ s⁻¹ at 298 K (review, Atkinson 1985)

$k_{OH} = (60.7 - 90.1) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (review, Atkinson 1989)

$k_{OH} = 6.10 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ with an estimated atmospheric lifetime of 2.3 h during summer daylight hours (Altshuller 1991)

$k_{OH} = 6.1 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, and $k_{O3} = 16.0 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime τ ~ 2.3 h, based on the photooxidation rate constant k = 6.10×10^{-11} cm³ molecule⁻¹ s⁻¹ with hydroxyl radical in air during summer daylight (Altshuller 1991).

Surface water: $t_{1/2}$ = 320 h and 9×10^4 d for reaction with OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2}$ = 7.3 d, based on oxidation reaction rate constant of 3×10^3 M⁻¹ s⁻¹ with singlet oxygen for unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.3.1
Reported aqueous solubilities of 2-methyl-1-butene at various temperatures

Pavlova et al. 1966	
Shake flask-GC	
t/°C	S/g·m⁻³
20	215
40	326
50	250
60	267
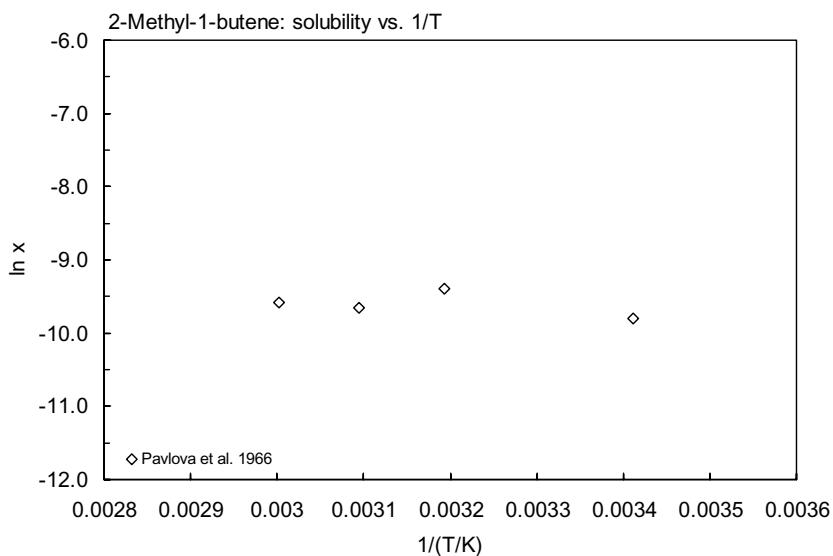
FIGURE 2.1.2.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-1-butene.

TABLE 2.1.2.1.3.2

Reported vapor pressures of 2-methyl-1-butene 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·log (T/K)	(4)

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

| Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971			
summary of literature data		ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–89.1	133.3	1.155	31163	–53.4	1333	eq. 2	P/mmHg
–72.8	666.6	6.054	38547	–43.7	2666	A	6.87314
–64.3	1333	10.993	47357	–37.5	4000	B	1053.780
–54.8	2666	15.973	57800	–32.87	5333	C	232.788
–44.1	5333	20.996	70242	–29.13	6666	bp/°C	31.163
–37.3	7999	26.062	84534	–25.96	7999	ΔH$_V$/(kJ mol^{-1}) =	
–28.0	13332	31.162	101319	–20.76	10666	at 25°C	25.86
–13.8	26664	36.308	120792	–16.54	13332	at bp	25.50
2.5	53329	41.500	143281	–8.44	19998		
20.2	101325	46.728	169952	–2.308	26664		
		52.005	198556	2.683	33331		
mp/°C	–135	57.320	232100	6.924	39997		
		62.675	270083	13.936	53329		
				19.865	66661		
		bp/°C	31.16	24.546	79993		
		Antoine eq.		28.623	93326		
		eq. 2	P/mmHg	29.620	95992		
		A	6.87314	30.400	98659		
		B	1052.780	31.163	101325		
		C	232.788	25.0	81327		
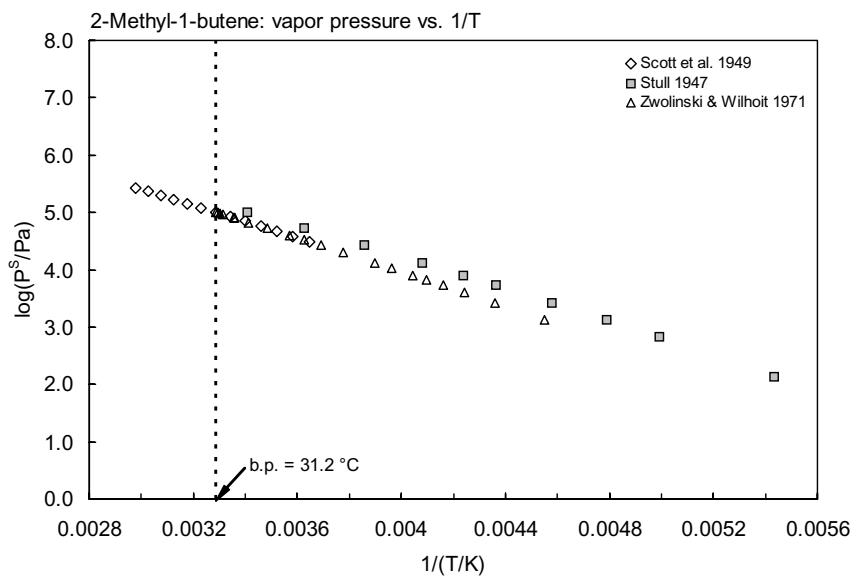
FIGURE 2.1.2.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1-butene.

2.1.2.1.4   3-Methyl-1-butene

Common Name: 3-Methyl-1-butene
Synonym:
Chemical Name: 3-methyl-1-butene
CAS Registry No: 563-45-1
Molecular Formula: C_5H_{10}, $(CH_3)_2CCHCH=CH_2$
Molecular Weight: 70.133
Melting Point (°C):
    –168.43   (Lide 2003)
Boiling Point (°C):
    20.1   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6272, 0.6219   (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
    111.8   (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)
    111.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.36   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    51.19, 41.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    130   (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    101325   (20.2°C, summary of literature data, temp range –89.1 to 20.2°C, Stull 1947)
    120790*   (25.128°C, ebulliometry, measured range 0.218–51.139°C, Scott & Waddington 1950)
    log (P/mmHg) = 6.82618 – 1013.474/(236.816 + t/°C); temp range 0.219–51.139°C (Antoine eq., ebulliometric method, Scott & Waddington 1950)
    120260   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.82618 – 1013.474/(237.0 + t/°C); temp range –47 to 60°C (Antoine eq. for liquid state, Dreisbach 1959)
    120000   (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    120270*   (derived from compiled data, temp range –62.9 to 40.84°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.82618 – 1013.474/(236.816 + t/°C); temp range –62.9 to 40.84°C (Antoine eq., Zwolinski & Wilhoit 1971)
    120180   (interpolated-Antoine eq., temp range –63 to 41°C, Dean 1985, 1992)
    log (P/mmHg) = 6.82455 – 1012.37/(236.65 + t/°C); temp range –63 to 41°C (Antoine eq., Dean 1985, 1992)
    120300   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.94656 – 1010.866/(–36.694 + T/K); temp range 237–324 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 31.1486 – 2.1764 × 10³/(T/K) –8.6146·log (T/K) + 5.9672 × 10⁻¹¹·(T/K) + 4.7555 × 10⁻⁶·(T/K)²; temp range 105–450 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    54230   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    63715, 22610   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    54700   (calculated-P/C, Mackay & Shiu 1981)
    43080   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

52940   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

     2.07   (calculated-regression of Lyman et al. 1982, Wang et al. 1992)

     2.05   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

     Volatilization:

     Photolysis:

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

         $k_{OH} = (3.10 \pm 0.31) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 299.2 K, measured range 299–433 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

         $k_{O(3P)} = 4.30 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom (Singleton & Cvetanovic 1976; quoted, Gaffney & Levine 1979)

         $k_{OH} = 3.18 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

         $k_{OH} = 9.01 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} and 6.07×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1985)

         $k_{OH}* = 3.18 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990)

         $k_{NO3} = 9.8 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1991)

         $k_{OH}* = 3.18 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 11.0 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 4.15 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

     Hydrolysis:

     Biodegradation:

     Biotransformation:

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

Half-Lives in the Environment:

     Surface water: $t_{1/2} = 320$ h and 9×10^4 d for reaction with OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on oxidation reaction rate constant $k = 3 \times 10^3$ M^{-1} s^{-1} with singlet oxygen for (unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.4.1

Reported vapor pressures of 3-methyl-1-butene 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)		

Scott & Waddington 1950				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0.210	47363	bp/°C	20.06	–62.9	1333	17.757	93326
5.112	57799	Antoine eq.		–53.4	2666	18.541	95992
10.053	70109	eq. 2	P/mmHg	–47.3	4000	19.309	98659
15.033	84158	A	6.82618	–42.6	5333	20.061	101325
20.061	101325	B	1913.474	–39.2	6666	25.0	120270
25.128	120790	C	236.816	–36.05	7999		
30.245	143268			–30.96	10666	eq. 2	P/mmHg
35.402	169066			–26.82	13332	A	6.82618
40.602	198543			–18.87	19998	B	1013.474
45.847	232073			–12.85	26664	C	236.816
51.139	280097			–7.95	33331	bp/°C	20.061
				–3.783	39997	ΔH_v/(kJ mol^{-1}) =	
				3.109	53329	at 25°C	23.85
				8.743	66661	at bp	24.06
				13.546	79993		
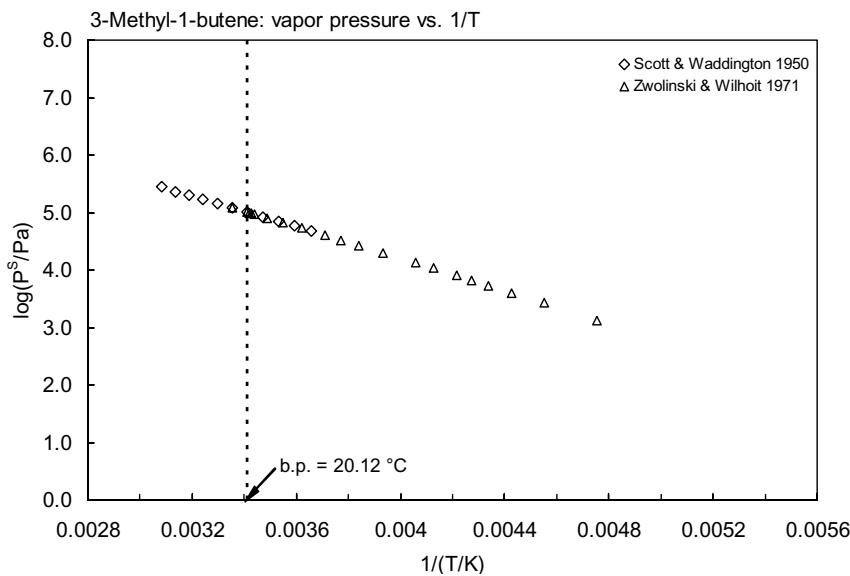
FIGURE 2.1.2.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methyl-1-butene.

2.1.2.1.5   2-Methyl-2-butene

Common Name: 2-Methyl-2-butene
Synonym:
Chemical Name: 2-methyl-2-butene
CAS Registry No: 513-35-9
Molecular Formula: C_5H_{10}, $CH_3CH=C(CH_3)CH_3$
Molecular Weight: 70.133
Melting Point (°C):
    –133.72   (Lide 2003)
Boiling Point (°C):
    38.56   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6623, 0.6570   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    105.9, 106.8 (20°C, 25°C, calculated-density)
    111.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.60   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    54.47, 59.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
    215*   (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
    325*   (calculated-liquid-liquid equilibrium LLE data, temp range 288–333.2 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    47876*   (18.07°C, static method, measured range –78.85 to 18.07°C, Lamb & Roper 1940)
    log (P/mmHg) = 9.86840 – 1773.506/(T/K) + 0.0035747·log (T/K); temp range –78.85 to 18.07°C (static method, Lamb & Roper 1940)
    53329*   (21.6, summary of literature data, temp range –75.4 to 38.5°C, Stull 1947)
    57798*   (ebulliometry, measured range 3.042 to 70.59°C, Scott et al. 1949)
    log (P/mmHg) = 6.91562 – 1095.088/(232.842 + t/°C); temp range 3.042 to 70.59°C (Antoine eq., ebulliometry, Scott et al. 1949)
    62140   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.91562 – 1095.088/(233.0 + t/°C); temp range –31 to 85°C (Antoine eq. for liquid state, Dreisbach 1959)
    62142*, 62140   (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.91562 – 1095.088/(232.842 + t/°C); temp range –47.7 to 60.0°C (Antoine eq., Zwolinski & Wilhoit 1971)
    62890, 62140   (calculated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.15017 – 1146.28/(238.416 + t/°C); temp range –78.85 to 18.07°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    log (P/kPa) = 6.04808 – 1099.054/(233.314 + t/°C); temp range 3.04–70.59°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    62240   (interpolated-Antoine eq., Dean 1985, 1992)
    log (P/mmHg) = 6.96659 – 1124.33/(236.63 + t/°C); temp range –48 to 60°C (Antoine eq., Dean 1985, 1992)
    62170   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.04475 – 1097.501/(–39.985 + T/K)$; temp range 271–343 K (Antoine eq., Stephenson & Malanowski 1987)

log $(P/mmHg) = 33.7539 – 2.426 \times 10^3/(T/K) – 9.4429 \cdot \log (T/K) + 9.8488 \times 10^{-11} \cdot (T/K) + 4.7156 \times 10^{-6} \cdot (T/K)^2$; temp range 139–471 K (vapor pressure eq., Yaws 1994)

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

24650   (calculated-P/C from selected data)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O3} = 7.47 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{OH} = 11.9 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{O(3P)} = 5.4 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} for reaction with O(^{3}P) (Herron & Huie 1973; Furuyama et al. 1974; Atkinson & Pitts Jr. 1978; quoted, Gaffney & Levine 1979)

$k_{O3} = 4.93 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} at 299 K (Japar et al. 1974)

$k_{OH} = 4.8 \times 10^9$ L mol^{-1} s^{-1} with atmospheric $t_{1/2} < 0.24$ h (Darnall et al.1976, Lloyd et al. 1976)

$k_{OH} = 8.4 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

$k_{OH} = 8.4 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}; $k_{O(3P)} = 54 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at room temp. (LFE correlation, Gaffney & Levine 1979)

$k_{OH} = (87.1 \pm 2.6) \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 297 ± 2 K (relative rate method, Ohta 1984)

$k_{NO3} = (5.5 \pm 1.2) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} 295 K (relative rate method, Atkinson et al. 1984a)

$k_{O3} = 4.2 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} with calculated lifetimes $\tau = 55$ min and 17 min in clean and moderately polluted atmosphere respectively, $k_{OH} = 8.7 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} with calculated lifetimes $\tau = 3.2$ h and 1.6 h in clean and moderately polluted atmosphere, respectively; $k_{NO3} = 5.5 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} with calculated lifetimes $\tau = 13$ min and 1.3 min in clean and moderately polluted atmosphere, respectively (Atkinson et al. 1984a)

$k_{NO2} < 0.5 \times 10^{-20}$ cm³ molecule^{-1} s^{-1} at 295 K (Atkinson et al. 1984b)

$k_{O3} = 4.5 \times 10^{-16}$ cm³ molecule^{-1} s^{-1}; $k_{OH} = 8.6 \times 10^{-11}$ cm³ molecule^{-1}s^{-1}; $k_{NO3} = 5.5 \times 10^{-12}$ cm³ molecule^{-1} s^{-1}; and $k_{O(3P)} = 47.6 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} with O(^{3}P) atom at room temp. (Atkinson et al. 1984b)

$k_{OH} = 8.68 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 295 ± 1 K (relative rate method, Atkinson & Aschmann 1984)

$k_{O3} = (6.79–7.97) \times 10^{-16}$ cm³ molecule^{-1} s^{-1}, 296–299 K (Atkinson & Carter 1984)

$k_{O3} = 4.2 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} with a loss rate of 25 d^{-1}; $k_{OH} = 8.7 \times 10^{-11}$ cm³ molecule^{-1}s^{-1} with a loss rate of 8 d^{-1}, and $k_{NO3} = 9.9 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} with a loss rate of 205 d^{-1} (Atkinson & Carter 1984)

$k_{OH} = 7.7 \times 10^{-11}$ to 1.19×10^{-10} cm³ molecule^{-1} s^{-1} between 297.7–299.5 K (Atkinson 1985)

$k_{O3} = 4.2 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} with a loss rate of 25 d^{-1}; $k_{OH} = 8.7 \times 10^{-11}$ cm³ molecule^{-1}s^{-1} with a loss rate of 3.8 d^{-1}, and $k_{NO3} = 9.9 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} with a loss rate of 205 d^{-1} at room temp (Atkinson 1985)

$k_{NO3} = (9.33 \pm 1.18) \times 10^{-12}$ cm³ molecule^{-1} s^{-1} 296 ± 2 K (relative rate method, Atkinson 1988)

$k_{OH} = 8.69 \times 10^{-11}$ cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 6.89 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}, $k_{O3} = 4.23 \times 10^{-16}$ cm³ molecule^{-1} s^{-1} at 198 K (Atkinson 1990)

$k_{OH} = 8.69 \times 10^{-11}$ cm³ molecule^{-1} s^{-1}, $k_{NO3} = 9.33 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 19 90)

$k_{NO3} = 9.37 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

$k_{OH}* = 8.69 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 9.37 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{O3}* = 4.03 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 5.1 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} < 0.24$ h, based on the photooxidation rate constant k = 4.8×10^9 L mol^{-1} s^{-1} with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976);

atmospheric lifetimes, τ(calc) = 0.95 h for the reaction with O$_3$, τ = 3.2 h with OH radical and τ = 0.12 h with NO$_3$ radical, based on the rate constants and environmental concentrations of OH, O$_3$ and NO$_3$ in the gas phase (Atkinson & Carter 1984);

calculated lifetimes: τ = 55 min due to reaction with O$_3$ in 24-h period, τ = 3.2 h with OH radical during daytime, and τ = 13 min for NO$_3$ radical during nighttime for "clean" atmosphere; τ = 17 min for reaction with O$_3$ in 24-h period, τ = 1.6 h with OH radical during daytime, and τ = 1.3 min with NO$_3$ radical during nighttime in "moderately" polluted atmosphere (Atkinson et al. 1984a);

atmospheric lifetimes τ(calc) = 6.38 h for the reaction with OH radical, τ(calc) = 0.92 h with O$_3$ and τ(calc) = 0.12 h with NO$_3$ radical in the gas phase (Atkinson 1985).

Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for reaction with OH and RO$_2$ radicals respectively in aquatic system, and $t_{1/2}$ = 8.0 d, based on rate constant of 10^6 M^{-1} s^{-1} for the reaction with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.5.1
Reported aqueous solubilities of 2-methyl-2-butene at various temperatures

Pavlova et al. 1966		Góral et al. 2004	
shake flask-GC		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	215	15	343
40	236	20	334
50	250	25	325
60	267	40	325
		50	338
		60	361
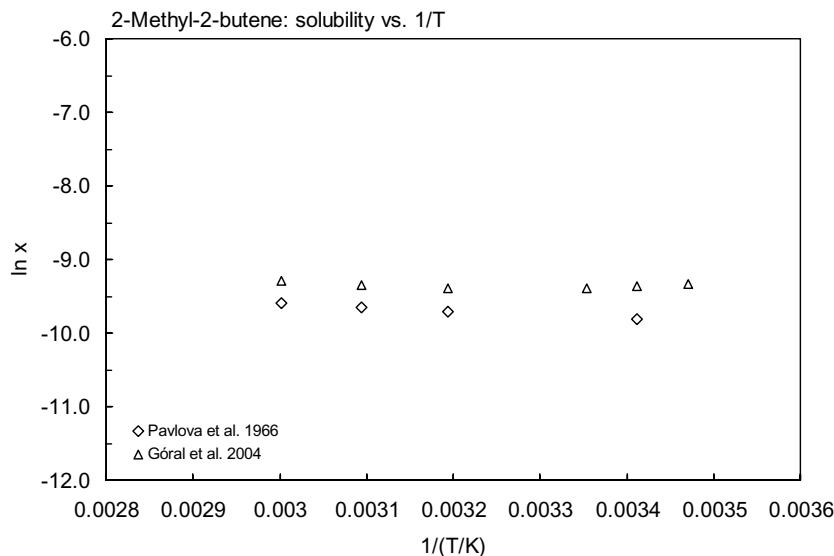
FIGURE 2.1.2.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-2-butene.

TABLE 2.1.2.1.5.2

Reported vapor pressures of 2-methyl-2-butene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)	$\ln P = A - B/(T/K)$ (1a)	
$\log P = A - B/(C + t/°C)$ (2)	$\ln P = A - B/(C + t/°C)$ (2a)	
$\log P = A - B/(C + T/K)$ (3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)		
$\log P = A - B/(T/K) - C \cdot (T/K)$ (5)		

Lamb & Roper 1940		Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971	
Static method-manometer		Summary of literature data		Ebulliometry		Selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−78.85	97	−75.4	133.3	3.042	25007	−47.7	1333
−54.78	811	−57.0	666.6	8.008	31172	−37.8	2666
−37.98	2696	−47.0	1333	12.987	38534	−31.46	4000
−29.84	4517	−37.9	2666	18.033	47364	−26.75	5333
−21.06	7537	−26.7	5333	23.103	57798	−22.92	6666
−12.14	11767	−19.4	7999	28.220	70110	−19.68	7999
−3.98	18238	−9.9	13332	33.373	84522	−14.37	10666
0.0	21918	4.0	26664	38.567	101319	−10.06	13332
0.0	22025	21.6	53329	43.806	120810	−1.786	19998
2.44	24625	38.5	101325	49.078	143268	4.486	26664
4.51	27024			54.399	169079	9.559	33331
16.31	44783	mp/°C	−133	59.753	198543	13.883	39997
18.07	47876			65.151	232087	21.029	53329
				70.590	272230	26.864	66661
bp/°C	38.43					31.834	79993
eq. 5	P/mmHg					36.187	93326
A	9.68640					36.998	95992
B	1773.506					37.791	98659
C	0.0035747					38.568	101325

TABLE 2.1.2.1.5.2 *(Continued)*

Lamb & Roper 1940		Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971	
Static method-manometer		Summary of literature data		Ebulliometry		Selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						25.0	62142
						eq. 2	P/mmHg
						A	6.91562
						B	1095.088
						C	232.842
						bp/°C	38.568
						ΔH_V/(kJ mol^{-1}) =	
						at 25°C	27.06
						at bp	26.30
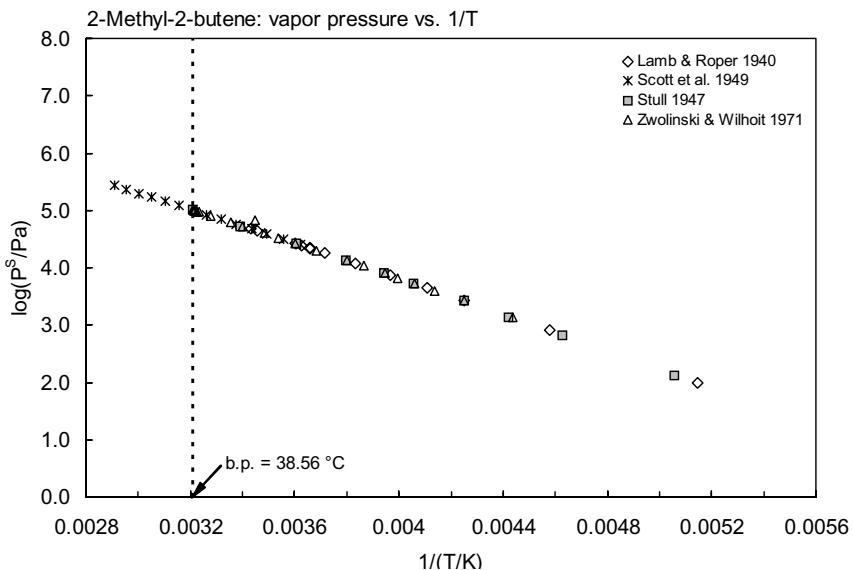
FIGURE 2.1.2.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-2-butene.

2.1.2.1.6   1-Pentene
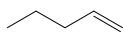
Common Name: 1-Pentene
Synonym: amylene, α-*n*-amylene, propylethylene
Chemical Name: 1-pentene
CAS Registry No: 109-67-1
Molecular Formula: C_5H_{10}
Molecular Weight: 70.133
Melting Point (°C):
    –165.12   (Lide 2003)
Boiling Point (°C):
    29.96   (Lide 2003)
Density (g/cm³):
    0.6405, 0.63533 (20°C, 25°C, Forziati et al. 1950, Dreisbach 1959)
    0.6353   (20°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    109.5   (20°C, calculated-density, Stephenson & Malanowski 1987)
    111.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    25.47, 25.20 (25 °, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.998   (Riddick et al. 1986)
    5.81   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    53.82, 54.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    148   (shake flask-GC, McAuliffe 1966)
    191   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    91420*   (interpolated-Antoine eq. regression, temp range –80.4 to 30.1°C, Stull 1947)
    70834   (20°C, static method, measured range 0–200°C, Day et al. 1948)
    log (P/mmHg) = 7.40607 – 1372.194/(T/K); temp range 0–30°C (static method, Day et al. 1948)
    log (P/mmHg) = 7.31561 – 1342.407/(T/K); temp range 40–95°C (static method, Day et al. 1948)
    84508*   (ebulliometry, measured range –0.159 to 61.64°C, Scott et al. 1949)
    log (P/mmHg) = 6.85487 – 1049.00/(233.994 + t/°C); temp range –0.159 to 61.64°C (Antoine eq., ebulliometry, Scott et al. 1949)
    83750*   (24.6°C, ebulliometry-manometer, measured range 12.8–30.7°C, Forziati et al. 1950)
    log (P/mmHg) = 6.78568 – 1014.293/(229.783 + t/°C); temp range 12.8–30.7°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
    86500   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.84650 – 1044.9/(234.0 + t/°C); temp range –39 to 73°C (Antoine eq. for liquid state, Dreisbach 1959)
    85000*   (interpolated-Antoine eq., temp range –63 to 41°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.84650 – 1044.895/(233.516 + t/°C); temp range –63 to 41°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 6931.2/(T/K)] + 7.914969; temp range –80.4 to 30.1°C (Antoine eq., Weast 1972–73)
    85020   (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.9716 – 1045.212/(233.598 + t/°C); temp range 12.84–30.7°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

85200   (interpolated-Antoine eq., temp range –55 to 51°C, Dean 1985, 1992)

log (P/mmHg) = 6.84424 – 1044.015/(233.50 + t/°C); temp range –55 to 51°C (Antoine eq., Dean 1985, 1992)

85100   (literature average, Riddick et al. 1986)

log (P/kPa) = 5.96914 – 1044.01/(233.49 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

85040   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.96999 – 1043.962/(–39.767 + T/K); temp range 218–311 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 36.2741 – 2.4452 × 10^3/(T/K) –10.405·log (T/K) – 7.4629 × 10^{-11}·(T/K) + 5.4070 × 10^{-6}·(T/K)^2; temp range 110–465 K (vapor pressure eq., Yaws 1994)

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

40330   (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)

41140   (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

37520, 22610 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

40300   (calculated-P/C, Mackay & Shiu 1981)

37520   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

40405   (calculated-P/C, Eastcott et al. 1988)

40280   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

2.69   (calculated-f const., Yalkowsky & Morozowich 1980)

2.20   (calculated-MCI χ, Murray et al. 1975)

2.80   (selected, Müller & Klein 1992)

2.3970   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

2.0*   (20.29°C, from GC determined γ^∞ in octanol, measured range 20.29–50.2°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = 4.25 × 10^{-11} cm³ molecule^{-1} s^{-1} at 298 K (discharge flow system-MS, Morris & Niki 1971)

k_{O3} = 1.07 × 10^{-17} cm³ molecule^{-1} s^{-1} (Japar et al. 1974)

k_{O3} = 5.3 × 10^{-18} cm³ molecule^{-1} s^{-1}, 7.4 × 10^{-18} cm³ molecule^{-1} s^{-1}, and 1.07 × 10^{-17} cm³ molecule^{-1} s^{-1} (review, Atkinson & Carter 1984)

k_{OH} = 3.13 × 10^{-11} cm³ molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

k_{OH} = 3.14 × 10^{-11} cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH} = 3.14 × 10^{-11} cm³ molecule^{-1} s^{-1}, k_{O3} = 1.10 × 10^{-17} cm³ molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k_{O3} = 1.00 × 10^{-17} cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1994)

k_{OH} = 3.14 × 10^{-11} cm³ molecule^{-1} s^{-1}, k_{O3}* = 10.0 × 10^{-18} cm³ molecule^{-1} s^{-1}, and $k_{O(3P)}$ = 4.65 × 10^{-12} cm³ molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for olefins in aquatic system by oxidation with OH and RO_2 radicals; while $t_{1/2} = 7.3$ d based on rate constant $k = 3 \times 10^5$ M^{-1} s^{-1} for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.6.1

Reported vapor pressures of 1-pentene 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		Scott et al. 1949		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–80.4	133.3	–0.159	31168	12.834	53703	–54.8	1333
–63.3	666.6	4.751	38545	18.468	66797	–45.1	2666
–54.5	1333	9.706	47348	24.584	63754	–38.91	4000
–46.0	2666	14.706	57789	28.900	97645	–34.28	5333
–34.1	5333	19.750	70094	29.362	99227	–30.53	6666
–27.1	7999	24.834	84508	29.796	100727	–27.36	7999
–17.7	13332	29.967	101322	30.289	102453	–22.14	10666
–3.40	26664	35.142	120813	30.723	103988	–17.92	13332
12.8	53329	40.359	143295			–9.789	19998
30.1	101325	45.614	169079	bp/°C	29.968	–3.640	26664
		50.914	198557			1.368	33331
mp/°C		56.253	232061	eq. 2	P/mmHg	5.624	39997
		61.641	270071	A	6.78568	12.664	53329
				B	1014.294	18.416	66661
		bp/°C	29.97	C	229.783	23.319	79993
		Antoine eq.				27.616	93326
		eq. 2	P/mmHg			28.417	95992
		A	6.85487			29.201	98659
		B	1049.00			29.968	101325
		C	233.994			25.0	85020
						eq. 2	P/mmHg
						A	6.84650
						B	1044.895
						C	233.516
						bp/°C	29.968
						$\Delta H_V/(kJ\ mol^{-1}) =$	
						at 25°C	25.47
						at bp	25.20
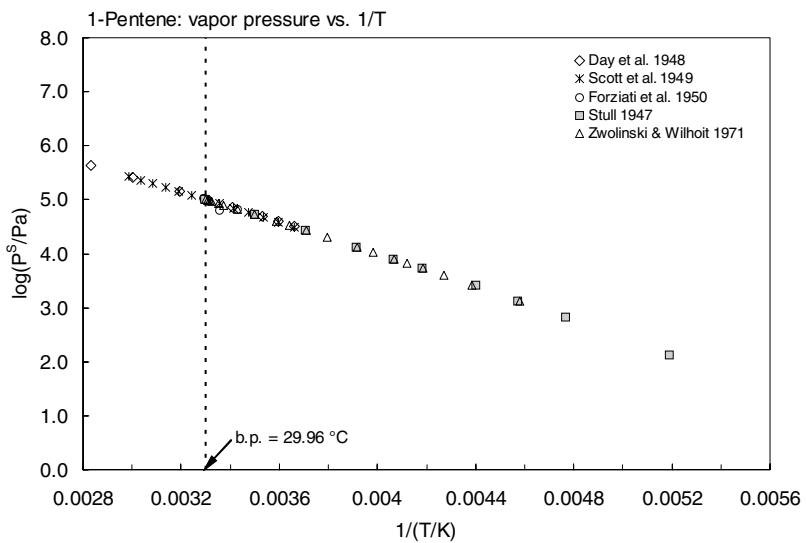
FIGURE 2.1.2.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1-pentene.

TABLE 2.1.2.1.6.2
Reported octanol-air partition coefficients of 1-pentene at various temperatures and temperature dependence equations

Gruber et al. 1997	
GC det'd activity coefficient	
t/°C	log K_{OA}
20.29	1.995
30.3	1.852
40.4	1.740
50.28	1.630
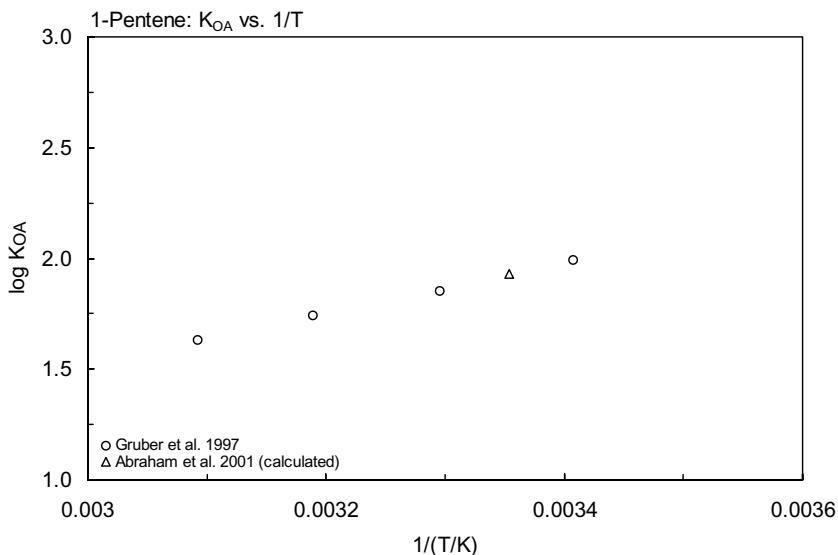
FIGURE 2.1.2.1.6.2 Logarithm of K_{OA} versus reciprocal temperature for 1-pentene.

2.1.2.1.7   cis-2-Pentene
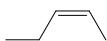
Common Name: *cis*-2-Pentene
Synonym: (*Z*)-2-pentene
Chemical Name: *cis*-2-pentene
CAS Registry No: 627-20-3
Molecular Formula: C_5H_{10}
Molecular Weight: 70.133
Melting Point (°C):
    –151.36   (Lide 2003)
Boiling Point (°C):
    36.93   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.6556, 0.6504 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
    107.0, 107.8 (20°C, 25°C, calculated-density)
    111.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.112   (Riddick et al. 1986)
    7.11   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    58.39, 52.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    203   (shake flask-GC, *cis-trans* form not specified, McAuliffe 1966)

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.):
    57795*   (21.541°C, ebulliometry, measured range 1.595–68.842°C, Scott & Waddington 1950)
    log (P/mmHg) = 6.87540 – 1069.460/(240.786 + t/°C); temp range 1.595–68.842°C (Antoine eq., ebulliometric method, Scott & Waddington 1950)
    65940   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.87274 – 1068.0/(231.0 + t/°C); temp range –33 to 82°C (Antoine eq. for liquid state, Dreisbach 1959)
    66000, 65941 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.87274 – 1067.951/(230.585 + t/°C); temp range –48.7 to 58.31°C (Antoine eq., Zwolinski & Wilhoit 1971)
    65950   (interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.99984 – 1069.227/(230.757 + t/°C); temp range 1.595–68.88°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    66640   (interpolated-Antoine eq., Dean 1985, 1992)
    66000   (quoted lit., Riddick et al. 1986)
    log (P/kPa) = 5.96798 – 1052.44/(228.693 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    log (P/mmHg) = 6.84308 – 1052.44/(228.69 + t/°C); temp range –49 to 58°C (Antoine eq., Dean 1985, 1992)
    65970   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P$_L$/kPa) = 5.99069 – 1064.178/(–43.035 + T/K); temp range 234–318 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 34.0427 – 2.4524 × 10^3/(T/K) –9.5014·log (T/K) – 5.0816 × 10^{-11}·(T/K) + 4.3638 × 10^{-6}·(T/K)^2; temp range 122–476 K (vapor pressure eq., Yaws 1994)

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

    22800   (calculated-P/C, Mackay & Shiu 1981)
    22770   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

    2.20   (calculated-π substituent constant, Hansch et al. 1968)
    2.20   (calculated-MCI χ, *cis-trans* form not specified, Murray et al. 1975)
    2.3772   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:
    Photolysis:
    Oxidation: 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:
        $k_{O(^3P)}$ = 1.80 × 10^{-11} cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom (Herron & Huie 1973; quoted,
            Gaffney & Levine 1979)
        k_{OH} = 6.20 × 10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)
        k_{OH} = (6.23 ± 0.1) × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Ohta 1984)
        k_{OH} = (65.4 – 65.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298–303 K (Atkinson 1989)
        k_{OH} = 6.50 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)
        k_{OH} = 6.50 × 10^{-11} cm^3 molecule^{-1} s^{-1} with an estimated atmospheric lifetime of 2.29 h in summer daylight
            (Altshuller 1991)
        k_{OH} = 6.5 × 10^{-11} cm^3 molecule^{-1} s^{-1}, and $k_{O(^3P)}$ = 1.7 × 10^{-11} cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom
            at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biodegradation:
   Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

    Air: photooxidation reaction rate constant k = 6.50 × 10^{-11} cm^3 molecule^{-1} s^{-1} with hydroxyl radical in air
        (Atkinson 1990, Altshuller 1991) with an estimated atmospheric lifetime of 2.29 h in summer daylight
        (Altshuller 1991).
    Surface water: $t_{1/2}$ ~ 320 h for oxidation by OH radicals, $t_{1/2}$ = 9 × 10^4 d for olefins in aquatic system, and $t_{1/2}$ =
        7.3 d based on rate constant k = 3 × 10^3 M^{-1} s^{-1} for oxidation of unsubstituted olefins by singlet oxygen in
        aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.7.1
Reported vapor pressures of *cis*-2-pentene at various temperatures

Scott & Waddington 1950

ebulliometric method

t/°C	P/Pa	t/°C	P/Pa
1.595	25009	58.070	198556
6.522	31163	63.456	232087
11.486	38546	68.882	270057
16.494	47357		
21.541	57795	log P = A − B/(C + t/°C)	
26.633	70102	bp/°C	36.94
31.766	84518		P/mmHg
36.944	101329	A	6.87540
42.161	120804	B	1069.460
47.423	143281	C	240.786
52.724	169066		

2.1.2.1.8   2-Methyl-1-pentene
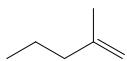
Common Name: 2-Methyl-1-pentene
Synonym:
Chemical Name: 2-methyl-1-pentene
CAS Registry No: 763-29-1
Molecular Formula: C_6H_{12}; $CH_3(CH_2)_2C(CH_3)CH_2$
Molecular Weight: 84.159
Melting Point (°C):
    –135.7   (Dreisbach 1959; Lide 2003)
Boiling Point (°C):
    60.7   (Dreisbach 1959)
    62.1   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6799, 0.6751   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    123.8, 124.7 (20°C, 25°C, calculated-density)
    133.2   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    78.0   (shake flask-GC, McAuliffe 1966)
    98.2   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    27464   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.88772 – 1154.7/(227.0 + t/°C); temp range –14 to 100°C (Antoine eq. for liquid state, Dreisbach 1959)
    26000, 26051 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.85030 – 1138.516/(224.764 + t/°C); temp range –30.1 to 85.16°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.85030 – 1138.516/(224.70 + t/°C); temp range –30 to 85°C (Antoine eq., Dean 1985, 1992)
    26060   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.89056 – 1091.679/(–46.306 + T/K); temp range 265–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.99434 – 1148.616/(–49.853 + T/K); temp range: 275–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = 32.9509 – 2.8171 × 10³/(T/K) –8.9572·log (T/K) – 8.7635 × 10⁻¹¹·(T/K) + 3.1710 × 10⁻⁶·(T/K)²; temp range 137–507 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    28100   (calculated-P/C, Mackay & Shiu 1981)
    28093   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
   Volatilization:
   Photolysis:
   Oxidation: 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:
      $k_{O3} = 1.05 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} under atmospheric conditions (Atkinson & Carter 1984)
      $k_{OH} = (8.76 \pm 0.14) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Ohta 1984)
      $k_{OH} = 62.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1985, Atkinson 1989)
      $k_{OH} = 6.3 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 15.0 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson
         1997)
   Hydrolysis:
   Biodegradation:
   Biotransformation:
   Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
   Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and
      $t_{1/2}$ = 8.0 d, based on rate constant k = 1.0×10^6 M^{-1} s^{-1} for oxidation of substituted olefins with singlet
      oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.1.9   4-Methyl-1-pentene
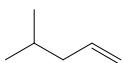
Common Name: 4-Methyl-1-pentene
Synonym:
Chemical Name: 4-methyl-1-pentene
CAS Registry No: 691-37-2
Molecular Formula: C_6H_{12}
Molecular Weight: 84.159
Melting Point (°C):
    –153.6   (Dreisbach 1959; Lide 2003)
Boiling Point (°C):
    53.88   (Dreisbach 1959)
    53.9   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6642, 0.6594 (20°C, 25°C, Dreisbach 1059)
Molar Volume (cm³/mol):
    126.7   (20°C, calculated-density, McAuliffe 1966, Ruelle & Kesselring 1997)
    127.6   (25°C, calculated-density)
    133.2   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    48.0   (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    35600   (calculated-Antoine eq., Dreisbach 1959)
    $\log (P/mmHg) = 6.87757 – 1130.0/(229.0 + t/°C)$; temp range –20 to 91°C (Antoine eq. for liquid state, Dreisbach 1959)
    36104, 36100 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    $\log (P/mmHg) = 6.83529 – 1121.302/(229.687 + t/°C)$; temp range –37.5 to 76.75°C (Antoine eq., Zwolinski & Wilhoit 1971)
    $\log (P/mmHg) = 6.83529 – 1121.302/(229.687 + t/°C)$; temp range –38 to 77°C (Antoine eq., Dean 1985, 1992)
    36110   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 5.94694 – 1114.082/(–44.332 + T/K)$; temp range 265–333 K (Antoine eq., Stephenson & Malanowski 1987)
    $\log (P/mmHg) = 44.7746 – 2.7364 \times 10^3/(T/K) – 14.283 \cdot \log (T/K) + 7.31 \times 10^{-3} \cdot (T/K) + 4.8402 \times 10^{-14} \cdot (T/K)^2$; temp range 120–496 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    62270   (calculated as $1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    65200, 34220 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    63200   (calculated-P/C, Mackay & Shiu 1981)
    63270   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    2.50   (calculated-π constant, Hansch et al. 1968)
    2.51   (calculated-MCI χ, Murray et al. 1975)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: 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:
        $k_{O3} = 1.06 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson & Carter 1984)
        $k_{O3} = 9.2 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
    Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and
        $t_{1/2}$ = 8.0 d, based on rate constant k = 1.0×10^6 M^{-1} s^{-1} for oxidation of substituted olefins with singlet
        oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.1.10   1-Hexene
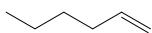
Common Name: 1-Hexene
Synonym: α-hexene
Chemical Name: 1-hexene
CAS Registry No: 646-04-8
Molecular Formula: C_6H_{12}; $CH_3(CH_2)_3CHCH_2$
Molecular Weight: 84.159
Melting Point (°C):
    –139.76   (Lide 2003)
Boiling Point (°C):
    63.48   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6732, 0.6685   (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    125.0   (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992; Ruelle & Kesselring 1997)
    125.9   (25°C, calculated-density)
    133.2   (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.347   (Riddick et al. 1986)
    9.35   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    70.1, 61.6   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
    50.0   (shake flask-GC, McAuliffe 1966)
    65.5   (shake flask-titration, Natarajan & Venkatachalam 1972)
    65.5, 54.12, 42.16 (25, 30, 35°C, shake flask-titration, in 0.001M HNO_3 solution, Natarajan & Venkatachalam 1972)
    55.4   (shake flask-GC, Leinonen & Mackay 1973)
    60.0   (20°C, shake flask-GC, Budantseva et al. 1976)
    69.7   (generate column-GC, Tewari et al. 1982a)
    100, 53   (20°C, 25°C, "best" values, IUPAC Solubility Data Series, Shaw 1989a)
    ln $x = -268.791 + 11353.70/(T/K) + 38.4871 \cdot$ ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)
    ln $x = -276.423 + 11833.54/(T/K) + 39.5126 \cdot$ ln (T/K); temp range 290–400 K (eq. derived from direct fit of solubility data, Tsonopoulos 2001)
    51.43*   (calculated-liquid-liquid equilibrium LLE data, temp range 293.2–494.3 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    22300*   (Antoine eq. regression, temp range –57.5 to 66°C, Stull 1947)
    23500*   (23.7°C, ebulliometry-manometer, measured range 15.9–64.3°C, Forziati et al. 1950)
    log (P/mmHg) = 6.86573 – 1152.971/(225.849 + t/°C); temp range 15.9–64.3°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
    25000   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.86572 – 1152.971/(226.0 + t/°C); temp range –12 to 79°C (Antoine eq. for liquid state, Dreisbach 1959)
    24800*, 24798 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.86573 – 1152.971/(225.849 + t/°C); temp range –29.3 to 86.64°C (Antoine eq., Zwolinski & Wilhoit 1971)

log $(P/mmHg) = [-0.2185 \times 7787.6/(T/K)] + 7.930324$; temp range -57.5 to $66°C$ (Antoine eq., Weast 1972–73)

24800   (interpolated-Antoine eq., Boublik et al. 1984)

log $(P/kPa) = 5.99426 - 1154.952/(226.002 + t/°C)$; temp range $15.89–64.311°C$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

24800   (interpolated-Antoine eq., temp range -16 to $64°C$, Dean 1985, 1992)

log $(P/mmHg) = 6.85770 - 1148.62/(225.25 + t/°C)$; temp range -16 to $64°C$ (Antoine eq., Dean 1985, 1992)

24800   (selected lit., Riddick et al. 1986)

log $(P/kPa) = 5.98260 - 1148.62/(225.346 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

24800   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log $(P_L/kPa) = 5.98336 - 1149.029/(-47.755 + T/K)$; temp range 273–343 K (Antoine eq., Stephenson & Malanowski 1987)

log $(P/mmHg) = 33.4486 - 2.6221 \times 10^3/(T/K) - 9.1784 \cdot \log (T/K) + 3.093 \times 10^{-12} \cdot (T/K) + 3.678 \times 10^{-6} \cdot (T/K)^2$; temp range 133–504 K (vapor pressure eq., Yaws 1994)

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

41750   (calculated-P/C, Mackay & Shiu 1975)

44080   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

51790, 34220   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

41800   (calculated-P/C, Mackay & Shiu 1981)

47230   (calculated-χ, Nirmalakhandan & Speece 1988)

41640   (calculated-P/C, Eastcott et al. 1988)

29940   (calculated-vapor–liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.39   (generator column-GC, Tewari et al. 1982a,b)

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

3.48   (calculated-activity coeff. γ, Wasik et al. 1982)

3.39, 3.40   (generator column-GC, calculated-activity coeff. γ, Schantz & Martire 1987)

3.40   (recommended, Sangster 1989)

3.39   (recommended, Hansch et al. 1995)

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

2.50*   (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O3} = 0.90 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Cadle & Schadt 1952)

$k_{O3} = 1.00 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Hanst et al. 1958)

$k_{O3} = 1.10 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{O3} = 1.40 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 296 K (static system-chemiluminescence, Cox & Penkett 1972)

$k_{O3} = 1.10 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 299 K (static system-chemiluminescence, Stedman et al. 1973)

$k_{O3} = 1.11 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ (static system-chemiluminescence, Japar et al. 1974)

$k_{O3} = 1.08 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (static system-chemiluminescence, Adeniji et al. 1981)

$k_{O3} = 1.21 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 296 K (static system-chemiluminescence, Atkinson et al. 1982)

$k_{O3} = (0.91$ to $1.36) \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 294–303 K (Atkinson & Carter 1984)

$k_{OH} = 3.68 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = (3.75 - 3.25) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 295–303 K (Atkinson 1985)

$k_{OH} = (32.9 - 37.5) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 295–303 K (Atkinson 1989)

$k_{OH} = 3.18 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 1.17 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

$k_{O3} = 1.10 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

$k_{OH} = 3.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{O3}* = 11.0 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 4.65 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on rate constant $k = 3 \times 10^3$ M^{-1} s^{-1} for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.10.1
Reported aqueous solubilities of 1-hexene at various temperatures

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Calc-recommended LLE data

t/°C	S/g·m^{-3}
20	56.11
25	51.43
36.8	51.43
93.3	102.9
148.8	392.8
204.4	2151
221.1	3740
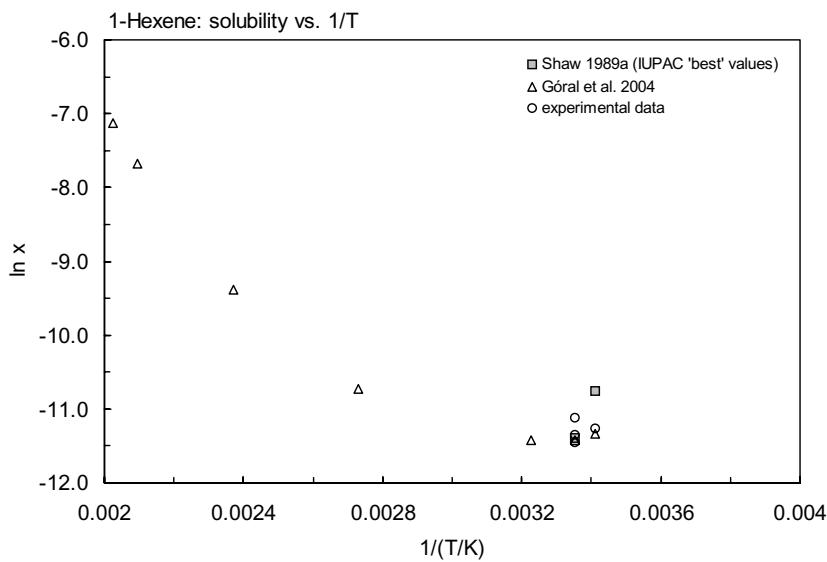
FIGURE 2.1.2.1.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-hexene.

TABLE 2.1.2.1.10.2
Reported vapor pressures and octanol-air partition coefficients of 1-hexene 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)		

Vapor pressure						$\log K_{OA}$	
Stull 1947		**Forziati et al. 1950**		**Zwolinski & Wilhoit 1971**		**Gruber et al. 1997**	
Summary of literature data		Ebulliometry		Selected values		GC det'd activity coefficient	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OA}
–57.5	133.3	15.890	16645	–29.30	1333	20.29	2.503
–38.0	666.6	19.950	19946	–18.65	2666	30.3	2.331
–28.1	1333	23.720	23485	–11.88	4000	40.4	2.20
–17.2	2666	28.762	28990	–6.81	5333	50.28	2.068
–5.0	5333	33.399	34936	–2.70	6666		
2.8	7999	38.993	43366	0.776	7999		
13.0	13332	44.763	53705	8.482	10666		
29.0	26664	50.914	66798	11.109	13332		
46.8	53329	62.323	97648	20.006	19998		
66.0	101325	62.827	99230	26.736	26664		
		63.299	100730	32.215	33331		
mp/°C		62.837	102457	38.871	39997		
		64.311	103995	44.569	53329		
				50.859	66661		
		eq. 2	P/mmHg	56.219	79993		
		A	6.86573	60.915	93326		
		B	1152.971	61.790	95992		
		C	225.849	62.647	98659		
		bp/°C	63.485	63.585	101325		
				25.0	24798		
				eq. 2	P/mmHg		
				A	6.86572		
				B	1152.971		
				C	225.849		
				bp/°C	63.485		
				$\Delta H_V/(kJ \; mol^{-1}) =$			
				at 25°C	28.28		
				at bp	30.63		
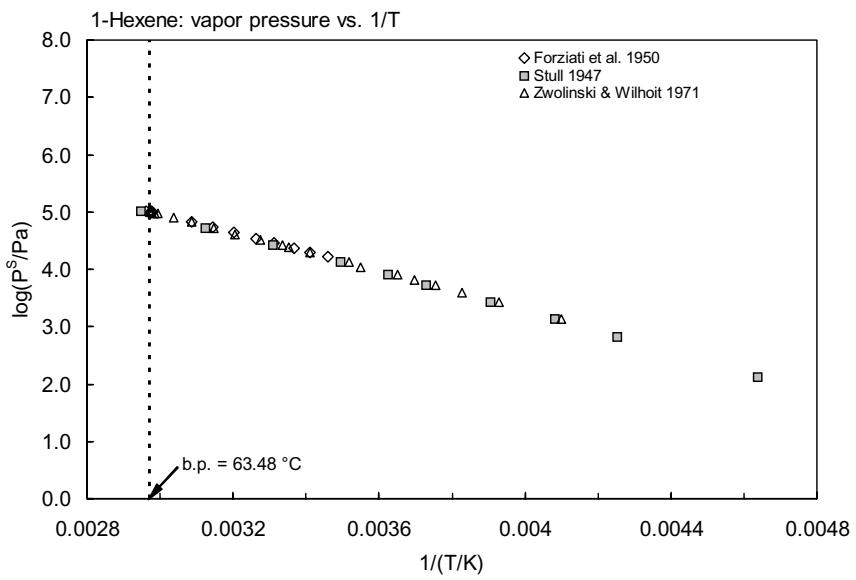
FIGURE 2.1.2.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexene.
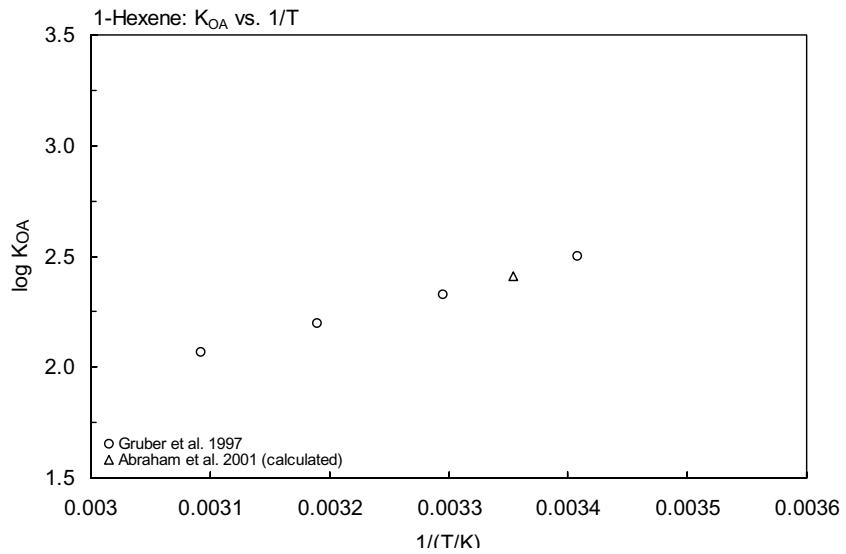
FIGURE 2.1.2.1.10.3 Logarithm of K_{OA} versus reciprocal temperature for 1-hexene.

2.1.2.1.11   1-Heptene
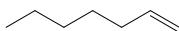
Common Name: 1-Heptene
Synonym: 1-heptylene, α-heptene
Chemical Name: 1-heptene
CAS Registry No: 592-76-7
Molecular Formula: C_7H_{14}, $CH_3(CH_2)_4CH=CH_2$
Molecular Weight: 98.186
Melting Point (°C):
    –118.9   (Lide 2003)
Boiling Point (°C):
    93.64   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6970, 0.6927   (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959)
Molar Volume (cm³/mol):
    140.9   (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
    141.8   (25°C, calculated-density)
    155.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    35.65, 31.09 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    12.401   (Riddick et al. 1986)
    12.66   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    82.5, 77.5   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
    Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    31.03, 27.6, 24.06 (20°C, 25°C, 30°C, shake flask-titration, in 0.001M HNO_3 solution, Natarajan & Venkatachalam 1972)
    18.16   (generator column-GC, Tewari et al. 1982a)
    23.6   (calculated-activity coeff. γ and K_{OW}, Tewari et al. 1982b)
    19, 25, 32, 38 (10, 20, 24, 30°C, "best values", IUPAC Solubility Data Series, Shaw 1989a)
    15.27, 13.6, 13.1 (10, 20, 30°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    7690*   (25.5°C, ebulliometry-manometer, measured range 21.6–94.5°C, Forziati et al. 1950)
    log (P/mmHg) = 6.90069 – 1257.505/(219.179 + t/°C); temp range 21.6–94.5°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
    7510   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.90069 – 1257.505/(219.18 + t/°C); temp range 10–128°C (Antoine eq. for liquid state, Dreisbach 1959)
    26663* (53.17°C, temp range 53.17–93.61°C, Eisen & Orav 1970; quoted, Boublik et al. 1984)
    7506*, 7510 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.90069 – 1257.505/(219.179 + t/°C); temp range –6.07 to 118.44°C (Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = [–0.2185 × 8643.2/(T/K)] + 7.991519; temp range –35.8 to 98.5°C (Antoine eq., Weast 1972–73)
    7520, 7530 (interpolated-Antoine equations., Boublik et al. 1984)
    log (P/kPa) = 6.04107 – 1266.473/(220.202 + t/°C); temp range 21.6–94.53°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

log (P/kPa) = 6.03512 – 1263.343/(219.922 + t/°C); temp range 54.17–93.61°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

7515   (interpolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.91087 – 1258.345/(219.30 + t/°C); temp range –6 to 118°C (Antoine eq., Dean 1985, 1992)

7500   (quoted lit., Riddick et al. 1986)

log (P/kPa) = 6.02677 – 1258.34/(219.299 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

7500   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99079 – 1237.44/(–56.26 + T/K); temp range 311–368 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 38.1255 – 3.064 × 10^3/(T/K) – 10.679·log (T/K) + 1.2244 × 10^{-10}·(T/K) + 3.668 × 10^{-6}·(T/K)^2; temp range 154–537 K (vapor pressure eq., Yaws 1994)

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

40580   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

3.99   (generator column-concn. ratio-GC, Tewari et al. 1982a,b)

4.09   (calculated-activity coeff. γ, Wasik et al. 1982)

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

3.99   (recommended, Sangster 1989, 1993)

3.99   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{O3} = 8.1 × 10^{-18} cm³ molecule^{-1} s^{-1} at room temp. (Cadle & Schadt 1952)

k_{O3} = 1.73 × 10^{-17} cm³ molecule^{-1} s^{-1} at 296 K (static system-chemiluminescence, Atkinson et al. 1982)

k_{OH} = 3.97 × 10^{-11} cm³ molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

k_{OH} = 40.5 × 10^{-12} cm³ molecule^{-1} s^{-1} and 36.1 × 10^{-12} cm³ molecule^{-1} s^{-1} at 298 K and 305 K respectively (Atkinson 1989)

k_{OH} = 4.0 × 10^{-11} cm³ molecule^{-1} s^{-1}, k_{O3} = 1.73 × 10^{-17} cm³ molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k_{OH} = 4.0 × 10^{-11} cm³ molecule^{-1} s^{-1}, k_{O3} = 12.0 × 10^{-18} cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2}$ ~ 320 h and 9 × 10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2}$ = 7.3 d, based on rate constant k = 3 × 10^3 M^{-1} s^{-1} for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.11.1
Reported vapor pressures of 1-heptene 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)		

Forziati et al. 1950		Eisen & Orav 1970		Zwolinski & Wilhoit 1971			
Ebulliometry		in Boublik et al. 1984		Selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
21.609	6485	53.17	26663	–6.07	1333	eq. 2	P/mmHg
25.492	7691	65.06	39997	5.39	2666	A	6.90069
28.768	8991	73.32	53329	12.68	4000	B	1257.505
34.525	11700	80.07	66661	18.15	5333	C	219.179
38.281	13845	85.82	79993	22.569	6666	bp/°C	93.643
42.564	16644	90.86	93325	26.306	7999		
46.923	19945	91.33	94659	32.443	10666	$\Delta H_V/(kJ\ mol^{-1})$ =	
50.970	23482	91.79	95992	37.418	13332	at 25°C	31.09
56.384	28988	92.25	97325	46.982	19998	at bp	35.65
67.366	43366	92.71	98658	54.212	26664		
73.563	53705	93.16	99991	60.096	33331		
80.179	66801	93.61	101325	65.095	39997		
92.391	97650			73.357	53329		
92.941	99233			80.104	66661		
93.444	100733			84.853	79993		
94.022	102462			90.888	93326		
94.531	104002			91.826	95992		
				92.744	98659		
eq. 2	P/mmHg			93.643	101325		
A	6.90069			25.0	7506		
B	1257.505						
C	219.179						
bp/°C	93.643						
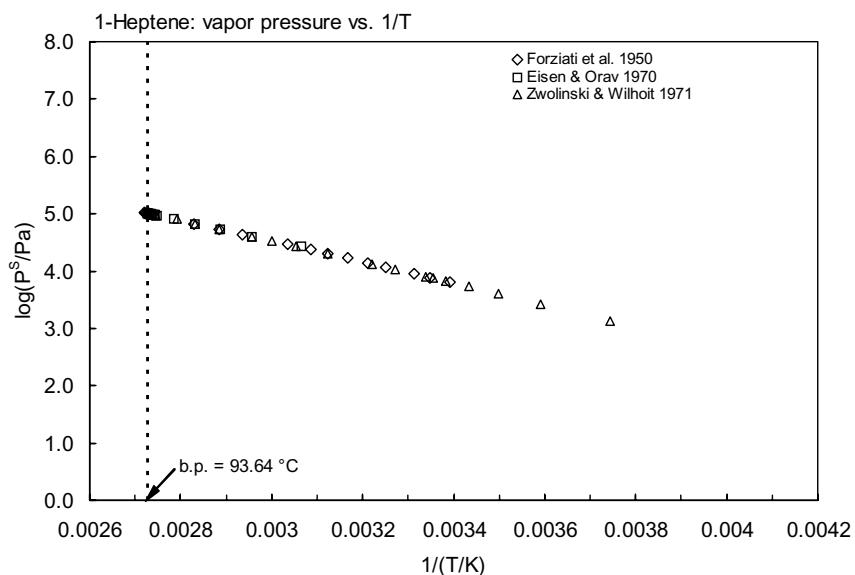
FIGURE 2.1.2.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 1-heptene.

2.1.2.1.12   1-Octene

Common Name: 1-Octene
Synonym: α-octene, caprylene, α-octylene
Chemical Name: 1-octene
CAS Registry No: 111-66-0
Molecular Formula: C_8H_{16}; $CH_3(CH_2)_5CH=CH_2$
Molecular Weight: 112.213
Melting Point (°C):
    –101.7   (Lide 2003)
Boiling Point (°C):
    121.29   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7149, 0.7109   (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    154.9   (20°C, calculated-density, Stephenson & Malanowski 1987)
    177.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    40.35, 33.95 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    15.569   (Riddick et al. 1986)
    15.31   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    89.29,86.8   (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    2.70   (shake flask-GC, McAuliffe 1966)
    4.10   (generator column-GC, Tewari et al. 1982a)
    6.82   (calculated-activity coeff. γ and K_{OW}, Tewari et al. 1982b)
    2.70, 22.2   (quoted, IUPAC Solubility Data Series, Shaw 1989)
    2.93, 2.93   (25, 37.78°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    6382*   (44.893°C, ebulliometry, measured range 44.893–122.223°C, Forziati et al. 1950)
    log (P/mmHg) = 6.93262 – 1353.486/(212.765 + t/°C); temp range 44.8–122.2°C (Antoine eq., ebulliometry-
        manometer measurements, Forziati et al. 1950)
    2317   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.93263 – 1253.5/(212.764 + t/°C); temp range 0–151°C (Antoine eq. for liquid state, Dreisbach
        1959)
    2320*   (interpolated-Antoine eq., temp range 15.38–147.54°C, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.93263 – 1253.486/(212.764 + t/°C); temp range 15.38–147.54°C (Antoine eq., Zwolinski &
        Wilhoit 1971)
    2320   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.06421 – 1356.472/(213.099 + t/°C); temp range 44.89–122.2°C (Antoine eq. from reported exptl.
        data Forziati et al. 1950, Boublik et al. 1984)
    2320   (interpolated-Antoine eq., temp range 15–147°C, Dean 1985, 1992)
    log (P/mmHg) = 6.93495 – 1355.46/(213.05 + t/°C); temp range 15–147°C (Antoine eq., Dean 1985, 1992)
    2300   (quoted lit., Riddick et al. 1986)
    log (P/kPa) = 6.05985 – 1355.46/(213.054 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    2320   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.05178 – 1350.245/(–60.716 + T/K); temp range 317–400 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 56.1183 – 3.7657×10^3/(T/K) – 10.006·log (T/K) + 7.7387×10^{-3}·(T/K) – 1.3036×10^{-6}·(T/K)^2; temp range 171–567 K (vapor pressure eq., Yaws 1994)

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

91700   (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)

96440   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

101000, 75000 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

96400   (calculated-P/C, Mackay et al. 1981; Eastcott et al. 1988)

74860   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

63500   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

4.57   (generator column-GC, Tewari et al. 1982a)

4.76   (calculated-activity coeff. γ, Wasik et al. 1981, 1982)

4.56, 4.72 (generator column-GC, calculated-activity coeff. γ, Schantz & Martire 1987)

4.57   (recommended, Sangster 1989)

4.57   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{O3} = 8.1×10^{-18} cm³ molecule^{-1} s^{-1} for the reaction with ozone in air (Atkinson & Carter 1984)

k_{OH} = 4.0×10^{-11} cm³ molecule^{-1} s^{-1}, k_{O3} = 1.70×10^{-17} cm³ molecule^{-1} s^{-1}, and $k_{O(3P)}$ = 1.10×10^{-11} cm³ molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom in gas phase (Paulson & Seinfeld 1992)

k_{O3} = 14.0×10^{-18} cm³ molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2}$ = 7.3 d, based on rate constant k = 3×10^3 M^{-1} s^{-1} for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.12.1
Reported vapor pressures of 1-octene 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)	

| Forziati et al. 1950				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
44.893	6382	121.075	100743	15.38	1333	118.362	93326
48.975	7690	121.685	102474	27.57	2666	119.355	95992
52.140	8994	122.223	102019	35.33	4000	120.328	98659
55.581	10330			41.15	5333	121.2880	101325
58.557	11720	eq. 2	P/mmHg	45.848	6666	25.0	2320
62.557	13844	A	6.93262	49.820	7999		
67.096	16644	B	1353.486	56.343	10666	eq. 2	P/mmHg
71.736	19945	C	212.764	61.630	13332	A	6.93263
76.022	23482	bp/°C	121.280	71.789	19998	B	1353.486
81.779	2890			79.645	26664	C	212.764
87.053	34934			85.710	33331	bp/°C	121.280
93.428	43366			91.014	39997	ΔH_v/(kJ mol^{-1}) =	
106.997	66806			99.778	53329	at 25°C	37.95
119.967	97658			106.932	66661	at bp	33.76
120.539	99242			113.026	79993		
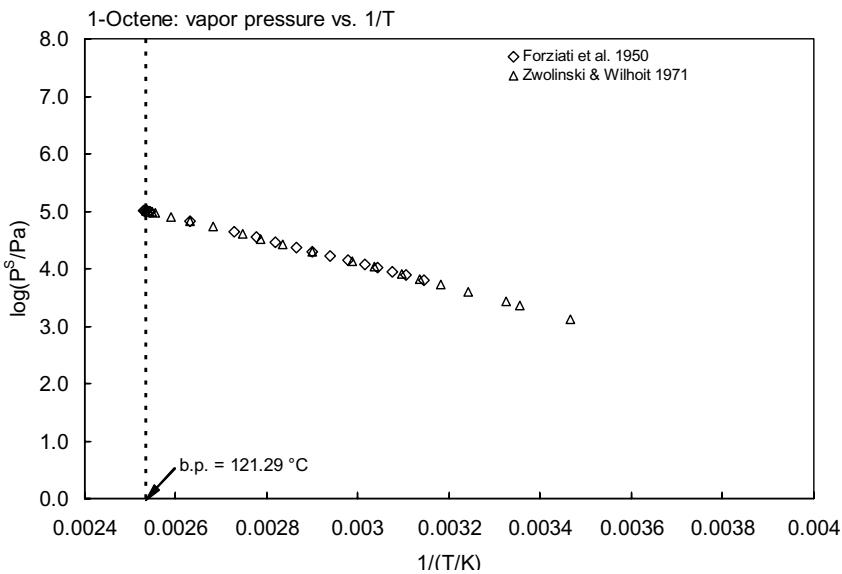
FIGURE 2.1.2.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-octene.

2.1.2.1.13   1-Nonene
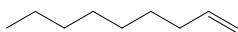
Common Name: 1-Nonene
Synonym: α-nonene, *n*-heptylethylene, 1-nonylene
Chemical Name: 1-nonene
CAS Registry No: 124-11-8
Molecular Formula: C_9H_{18}; $CH_3(CH_2)_6CH=CH_2$
Molecular Weight: 126.239
Melting Point (°C):
    –81.3   (Lide 2003)
Boiling Point (°C):
    146.9   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7292, 0.7235 (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
    173.1, 174.1 (20°C, 25°C, calculated-density)
    199.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    45.52, 36.31 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    19.075   (Riddick et al. 1986)
    19.37   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    104.23, 96.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.63   (estimated-nomograph, Brookman et al. 1986)
    1.12   (generator column-GC, Tewari et al. 1982a)
    2.09   (calculated-activity coeff. γ and K_{OW}, Tewari et al. 1982b)

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.):
    6385*   (66.607°C, ebulliometry, measured range 66.607–147.860°C, Forziati et al. 1950)
    log (P/mmHg) = 6.95389 – 1435.359/(205.535 + t/°C); temp range 66.6–147.9°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
    712   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.95387 – 1435.295/(205.535 + t/°C); temp range 25–173°C (Antoine eq. for liquid state, Dreisbach 1959)
    707*, 712 (derived from compiled data, extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.95430 – 1436.20/(205.69 + t/°C); temp range 35–175°C (Antoine eq., Dean 1985, 1992)
    710   (quoted lit., Riddick et al. 1986)
    log (P/kPa) = 6.07920 – 1436.20/(205.690 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    712   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.07341 – 1432,435/(–67.884 + T/K); temp range 339–423 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 60.6089 – 4.2023 × 10³/(T/K) – 19.446·log (T/K) + 7.8308 × 10⁻³·(T/K) + 1.591 × 10⁻¹³·(T/K)²; temp range 192–593 K (vapor pressure eq., Yaws 1994)
    650.4   (23.25°C, transpiration method, Verevkin et al. 2000)
    ln (P/Pa) = 24.60 – 5379/(T/K); temp range 278.5–318.3 K (transpiration method, Verevkin et al. 2000)

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

  80450   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

  5.15   (generator column-GC, Tewari et al. 1982a,b)
  5.34   (calculated-activity coeff. γ, Wasik et al. 1981, 1982)
  5.31   (calculated-activity coeff. γ, Schantz & Martire 1987)
  5.15   (recommended, Sangster 1989)
  5.15   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

  Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and
     $t_{1/2}$ = 7.3 d, based on rate constant k = 3×10^3 M^{-1} s^{-1} for oxidation of unsubstituted olefins with singlet
     oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.13.1

Reported vapor pressures of 1-nonene 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)	

Forziati et al. 1950				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.607	6385	146.091	99242	35.55	1333	143.805	93326
70.874	7691	146.653	100742	48.38	2666	144.848	95992
74.517	8994	147.289	102474	56.55	4000	145.869	98659
77.861	10331	147.860	104020	62.67	5333	146.868	101325
81.001	11722			67.612	6666	25.0	706.6
85.202	13805	bp/°C	146.868	71.790	7999		
89.942	16644			78.651	10666	eq. 2	P/mmHg
94.829	19945	eq. 2	P/mmHg	84.210	13332	A	6.95387
99.341	23482	A	6.95389	94.889	19998	B	1435.359
110.935	34934	B	1435.359	102.956	26664	C	205.535
117.622	43364	C	146.868	109.518	33331	bp/°C	146.868
124.521	53707			115.090	39997	ΔH_V/(kJ mol⁻¹) =	
131.881	66806			124.295	53329	at 25°C	36.32
139.859	83770			131.808	66661	at bp	45.52
145.488	97658			138.204	79993		
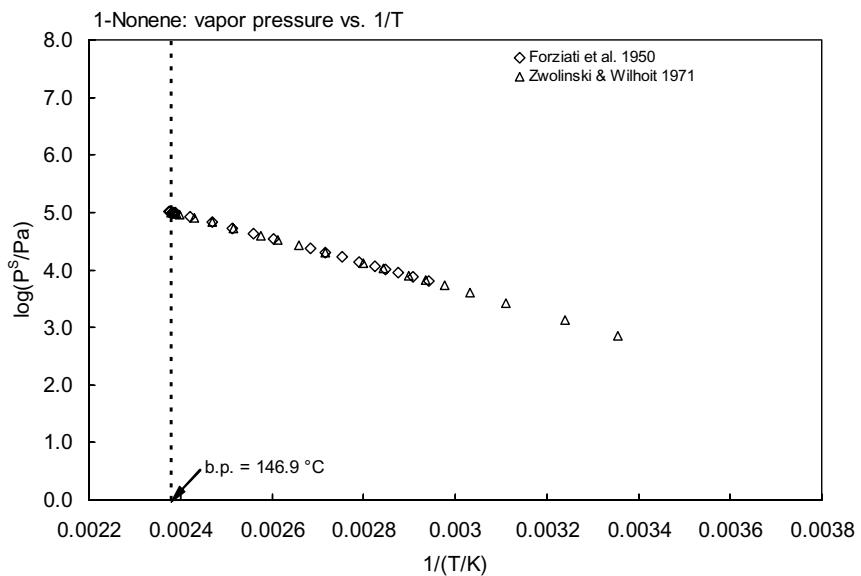
**FIGURE 2.1.2.1.13.1** Logarithm of vapor pressure versus reciprocal temperature for 1-nonene.

2.1.2.1.14   1-Decene
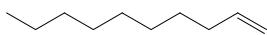
Common Name: 1-Decene
Synonym: α-decene
Chemical Name: 1-decene
CAS Registry No: 872-05-9
Molecular Formula: $C_{10}H_{20}$
Molecular Weight: 140.266
Melting Point (°C):
     –66.3   (Lide 2003)
Boiling Point (°C):
     170.5   (Lide 2003)
Density (g/cm³ at 20°C):
     0.7408, 0.7369 (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959)
Molar Volume (cm³/mol):
     189.3   (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
     190.3   (25°C, calculated-density)
     222.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     50.43, 38.66 (25°, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     21.75   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     106.8, 105.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
     5.70   (shake flask-titration with bromine, Natarajan & Venkatachalam 1972; quoted Shaw 1989)
     11.0, 8.50, 5.70 (15, 20, 25°C, shake flask-titration, in 0.001M HNO_3 solution, Natarajan & Venkatachalam 1972)
     0.161   (calculated-K_{OW}, Wang et al. 1992)
     0.433   (calculated-molar volume V_M, Wang et al. 1992)
     0.222, 0.344 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
     0.429, 4.29, 70.13 (101, 151.5, 202°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
     133.3*   (14.7°C, summary of literature data, temp range 14.7–192.0°C, Stull 1947)
     6397*   (86.774°C, ebulliometry, measured range 86.774–171.605°C, Forziati et al. 1950)
     log (P/mmHg) = 6.96036 – 1501.812/(197.578 + t/°C); temp range 86.7–171.6°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
     218   (calculated-Antoine eq., Dreisbach 1959)
     log (P/mmHg) = 6.96034 – 1501.872/(197.58 + t/°C); temp range 25–253°C (Antoine eq. for liquid state, Dreisbach 1959)
     218*   (extrapolated-Antoine eq., temp range 54.4–199.3°C, Zwolinski & Wilhoit 1971)
     log (P/mmHg) = 6.96034 – 1501.872/(197.578 + t/°C); temp range 54.4–199.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
     log (P/kPa) = 6.07985 – 1497.943/(197.102 + t/°C); temp range 86.77–171.6°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
     215   (extrapolated-Antoine eq., temp range: 54–199°C, Dean 1985, 1992)
     log (P/mmHg) = 6.93477 – 1484.98/(195.707 + t/°C), temp range: 54–199°C (Antoine eq., Dean 1985, 1992)
     210   (quoted lit., Riddick et al. 1986)

log (P/kPa) = 6.05967 – 1484.98/(195.707 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

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

log (P$_L$/kPa) = 6.12458 – 1528.811/(–72.566 + T/K); temp range 383–445 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 2.2678 – 3.1244 × 10^3/(T/K) + 5.432·log (T/K) – 2.0137 × 10^{-2}·(T/K) + 1.1221 × 10^{-5}·(T/K)^2; temp range 207–617 K (vapor pressure eq., Yaws 1994)

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

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

4.78   (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
5.18   (calculated-molar volume V$_M$, Wang et al. 1992)
4.7037   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

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

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

Volatilization:
Photolysis:
Oxidation: 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$_{O3}$ = 1.08 × 10^{-17} cm^3 molecule^{-1} s^{-1} for reaction with ozone in the gas phase (Atkinson & Carter 1984)
k$_{O3}$ = 9.3 × 10^{-18} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k$_1$) and Elimination (k$_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: t$_{1/2}$ ~ 320 h and 9 × 10^4 d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and t$_{1/2}$ = 7.3 d, based on rate constant k = 3 × 10^3 M^{-1} s^{-1} for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.14.1
Reported vapor pressures of 1-decene 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		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
14.7	133.3	86.774	6397	54.40	1333
40.3	666.6	91.308	7694	67.80	2666
53.7	1333	95.134	8997	76.33	4000
67.8	2666	98.604	10334	82.71	5333
83.3	5333	101.844	11723	87.875	6666

(*Continued*)

TABLE 2.1.2.1.14.1 (*Continued*)

Stull 1947		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
93.5	7999	106.223	13848	92.236	7999
14.7	133.3	86.774	6397	54.40	1333
106.5	13332	111.213	16647	99.396	10666
126.7	26664	116.283	19950	105.198	13332
149.2	53329	120.995	23463	116.342	19998
192.0	101325	127.265	28990	124.760	26664
		140.063	43759	131.607	33331
mp/°C		147.265	53710	137.421	39997
		154.939	66810	147.024	53329
		169.134	97662	154.861	66661
		169.762	99247	161.533	79993
		170.345	100747	163.376	93326
		171.012	102487	168.464	95992
		171.605	104026	170.052	98659
				170.570	101325
		eq. 2	P/mmHg		
		A	6.96036	eq. 2	P/mmHg
		B	1501.872	A	6.96034
		C	197.578	B	1501.872
		bp/°C	170.570	C	197.578
				bp/°C	170.570
				ΔH_V/(kJ mol^{-1}) =	
				at 25°C	38.66
				at bp	50.46
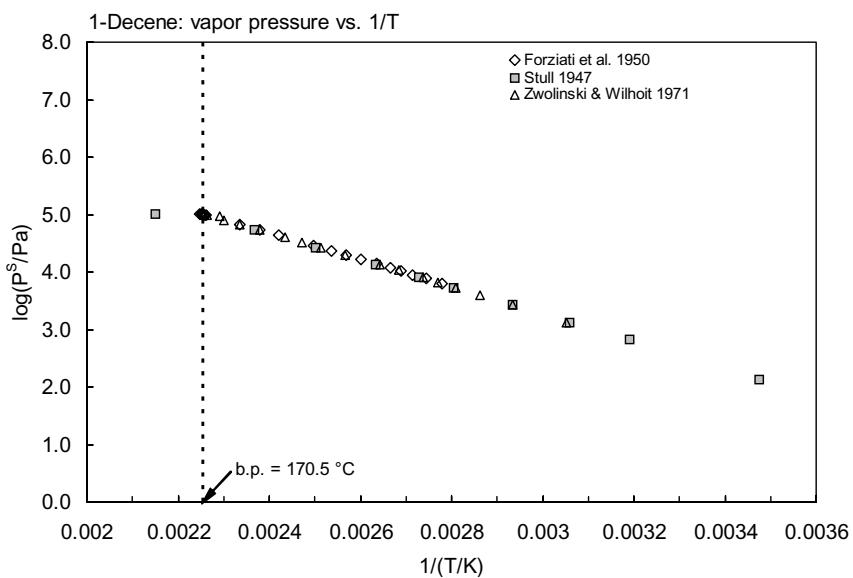
FIGURE 2.1.2.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for 1-decene.

2.1.2.2   Dienes

2.1.2.2.1   1,3-Butadiene

Common Name: 1,3-Butadiene
Synonym: α,γ-butadiene, bivinyl, divinyl, erythrene, vinylethylene, biethylene, pyrrolylene
Chemical Name: 1,3-butadiene
CAS Registry No: 106-99-0
Molecular Formula: C_4H_6; $CH_2=CHCH=CH_2$
Molecular Weight: 54.091
Melting Point (°C):
    –108.91   (Lide 2003)
Boiling Point (°C):
    –4.41   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6211, 0.6149 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
    87.1   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987; Wang et al. 1992
            Ruelle & Kesselring 1997)
    81.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.98   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    48.62, 45.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    735   (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

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.):
    113857*   (–1.50°C, static method-manometer, measured range –75.5 to –1.50°C, Heisig 1933)
    336200*   (calculated-Antoine eq. regression, temp range –102.8 to 4.6°C, Stull 1947)
    280600   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 6.85941 – 935.53/(239.55 + t/°C); temp range –66 to 46°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    281000*   (extrapolated-Antoine eq., temp range –58.201 to 14.43°C, Zwolinski & Wilhoit 1971)
    280644   (derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.84999 – 930.546/(238.854 + t/°C); temp range –58.201 to 14.43°C (Antoine eq., Zwolinski
        & Wilhoit 1971)
    61295*   (20.211°C, temp range –16.204 to 33.257°C, Boublikova 1972; quoted, Boublik et al. 1984)
    247700   (extrapolated-Antoine eq., temp range –82.5 to 9.7°C, Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 7761.0/(T/K)] + 8.997505; temp range –82.5 to 9.7°C (Antoine eq., Weast 1972–73)
    281650, 281510* (static method quartz manometer, measured range 15–55°C, Flebbe et al. 1982)
    281230, 310400(extrapolated-Antoine equations, Boublik et al. 1984)
    log (P/kPa) = 6.86369 – 1313.687/(275.492 + t/°C); temp range –81 to –24°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    log (P/kPa) = 5.97484 – 931.996/(239.329 + t/°C); temp range –75 to –1.5°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    log (P/mmHg) = 7.03555 – 998.106/(245.233 + t/°C); temp range –87 to –62°C (Antoine eq., Dean 1985, 1992)
    log (P/mmHg) = 6.84999 – 930.546/(238.854 + t/°C); temp range –58 to 15°C (Antoine eq., Dean 1985, 1992)
    281000   (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.16045 – 998.106/(–27.916 + T/K); temp range 193–213 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.97489 – 930.546/(–34.306 + T/K); temp range 213–276 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99667 – 940.687/(–33.017 + T/K); temp range 270–318 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.31615 – 1130.927/(–5.606 + T/K); temp range 315–382 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.86984 – 3877.451/(315.612 + T/K); temp range 380–425 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log $(P/mmHg)$ = 30.0572 – 1.9891 × 10³/(T/K) –8.2922·log (T/K) + 2.5664 × 10⁻¹⁰·(T/K) + 5.1334 × 10⁻⁶·(T/K)²; temp range 164–425 K (vapor pressure eq., Yaws 1994)

ln (P/atm) = 9.16107 – 2154.139/(T/K – 33.596); temp range 207–319 K (Antoine eq., Oliveira & Uller 1996)

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

7460	(calculated-P/C, Mackay & Shiu 1981)
6370	(calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1989)
7150, 6230	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
10820	(calculated-MCI χ, Nirmalakhandan & Speece 1988)
7720	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

1.99	(shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)
1.87, 1.68, 1.90	(calculated-fragment const., Rekker 1977)
2.22	(calculated-UNIFAC, Banerjee & Howard 1988)
1.99	(recommended, Sangster 1989)
1.56	(calculated-V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

1.28	(calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

1.86–2.36	(soils and sediments, calculated-K_{OW} and S, Lyman et al. 1982; quoted, Howard 1989)

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

Volatilization: volatilizes rapidly from water and land (Howard 1989).

Photolysis:

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

k_{O3} = 8.4 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ at 299 K (Japer et al. 1974)

k_{OH} = (46.4 ± 9.3) × 10⁹ L mol⁻¹ s⁻¹ at 305 ± 2 K (relative rate method, Lloyd et al. 1976)

k_{OH} = 4.64 × 10¹⁰ L mol⁻¹ s⁻¹, $t_{1/2}$ = 0.25 h for reaction with OH radical only, $t_{1/2}$ = 0.24 h with an average concn of 0.1 ppm of O_3 at 300 K (Darnall et al. 1976)

$k_{O(3P)}$ = 1.9 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for reaction with O(³P) atom at room temp. (Atkinson & Pitts, Jr. 1977)

k_{OH}* = (6.85 ± 0.69) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 299.5 K, measured range 299.9–424 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

k_{OH} = 6.9 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

k_{O3}* = (1.17 ± 0.19) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 296 K, measured range 276–324 K with atmospheric lifetime τ ~ 24 h due to reaction with O_3 and τ ~ 4 h with OH radical (Atkinson et al. 1982)

$k_{OH} = 6.85 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 297 ± K, k_{OH}(calc) = 6.22×10^{-11} cm^3 molecule^{-1} s^{-1} (relative rate method, Ohta 1983)

$k_{O3} = (6.1 - 8.4) \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at room temp. to 299 K (Atkinson & Carter 1984)

$k_{NO3} = (5.34 \pm 0.62) \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson et al. 1984a)

$k_{NO2} = (3.1 \pm 0.3) \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with NO$_2$ at 295 ± 2 K (relative rate method, Atkinson et al. 1984b)

$k_{OH} = 6.8 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 0.053 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 8.4 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}; $k_{O(3P)} = 6.4 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{NO2} = 3.1 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with NO$_2$, at room temp. (Atkinson et al. 1984b)

$k_{OH} = 6.65 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{NO3} = 2.1 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (fast flow system/MS, Benter & Schindler 1988)

$k_{OH}* = 6.66 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{NO3} = (4.4 \pm 0.8) \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 296 ± 1 K (FTIR, Andersson & Ljungström 1989)

$k_{OH} = 66.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 7.5 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} (Atkinson 1990)

$k_{NO3} = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

$k_{OH} = 6.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 7.5 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} (Sabljic & Gusten 1990)

$k_{OH} = 2.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, $k_{O3}* = 6.3 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 1.98 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis: will hydrolyze appreciably (Howard 1989).

Biodegradation: $t_{1/2}$(aerobic) = 7 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: estimated photooxidation $t_{1/2}$ = 0.24–24 h (Darnall et al 1976) for the reaction with hydroxyl radical; photooxidation with OH radicals with an estimated $t_{1/2}$ ~ 3.1 h (Lyman et al. 1982; quoted, Howard 1989); completely degraded within 6 h in a smog chamber irradiated by sunlight (Kopcynski et al 1972; quoted, Howard 1989);

$t_{1/2}$ = 15 h in air for the reaction with nitrate radical (Atkinson et al. 1984a; quoted, Howard 1989);

$t_{1/2}$ = 0.76–7.8 h, based on measured photooxidation rate constants in air (Howard et al. 1991).

Surface water: $t_{1/2}$ = 1200 to 48000 h, based on measured photooxidation rate constants with OH radicals in water (Güsten et al. 1981; quoted, Howard et al. 1991);

estimated $t_{1/2}$ = 3.8 h for evaporation from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2}$ ~ 320 h and $t_{1/2}$ = 9×10^4 for oxidation by OH and RO$_2$ radicals and $t_{1/2}$ = 9×10^4 d for olefins in aquatic system, and $t_{1/2}$ = 19 h, based on rate constant of 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985);

volatilizes rapidly with a half-life estimated to be several hours (Howard 1989);

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

$t_{1/2}$(aerobic) = 7 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995).

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

Sediment:

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

Biota:

TABLE 2.1.2.2.1.1
Reported vapor pressures of 1,3-butadiene 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)	
log P = A[1 – Φ /(T/K)]	(5) where log A = a + bT + cT²	

Heisig 1933		Stull 1947		Zwolinski & Wilhoit 1971		Flebbe et al. 1982	
static method-manometer		summary of literature data		selected values		static-quartz manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–75.5	1946	–102.8	133.3	–79.86	1333	15	144720
–63.4	4720	–87.6	666.6	–71.18	2666	15	144700
–51.6	10279	–79.7	1333	–65.676	4000	25	281650
–39.4	20452	–71.0	2666	–61.44	5333	25	281510
–38.6	21558	–61.3	5333	–58.201	6666	35	499680
–32.7	29197	–55.1	7999	–55.381	7999	35	499250
–26.1	40183	–46.8	13332	–50.747	10666	55	824250
–19.9	53395	–33.9	26664	–46.989	13332	55	823810
–15.5	64554	–19.3	53329	–39.760	19998		
–10.4	79980	–4.60	101325	–34.292	26664	vapor pressure eq. given	
–5.60	97285			–29.839	33331	in reference	
–1.50	113857	mp/°C	–108.0	–26.054	39997		
				–19.796	53329		
				–14.681	66661		
				–10.322	79993		
				–6.502	93326		
				–5.979	95992		
				–5.093	98659		
				–4.411	101325		
				25.0	280644		

eq. 2   P/mmHg
A   6.84999
B   930.546
C   238.854
temp range –58 to 14.4°C
bp/°C   –4.411
ΔH_V/(kJ mol⁻¹) =
at 25°C   21.05
at bp   22.68
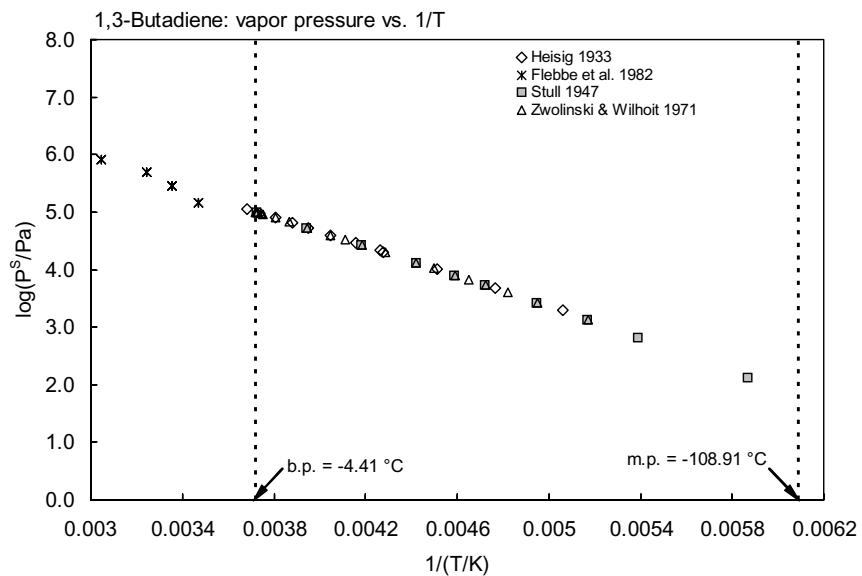
FIGURE 2.1.2.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3-butadiene.

2.1.2.2.2   2-Methyl-1,3-butadiene (Isoprene)

Common Name: 2-Methyl-1,3-butadiene
Synonym: isoprene
Chemical Name: 2-methyl-1,3-butadiene
CAS Registry No: 78-79-5
Molecular Formula: C_5H_8; $CH_2=C(CH_3)CH=CH_2$
Molecular Weight: 68.118
Melting Point (°C):
    –145.9   (Lide 2003)
Boiling Point (°C):
    34   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6809, 0.6759 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    100.4   (20°C, calculated-density)
    103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    4.92   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    38.68, 34.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section.):
    642   (shake flask-GC, McAuliffe 1966)
    545*   (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
    610*   (recommended best value, IUPAC Solubility Data Series, temp range 20–60°C, Shaw 1989a)
    530*   (calculated-liquid-liquid equilibrium LLE data, temp range 293.2–313.2 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    53329*   (15.4°C, summary of literature data, temp range –79.8 to 32.6°C, Stull 1947)
    66816*   (22.5°C, ebulliometry, measured range 16.8–34.8°C, Forziati et al. 1950)
    log (P/mmHg) = 6.90335 – 1080.996/(234.668 + t/°C); temp range 16.8–34.8°C (Antoine eq., ebulliometry
        measurements, Forziati et al. 1950)
    3349*   (–38.227°C, inclined-piston manometer, measured range –57.598 to –38.227°C, Osborn & Douslin
        1969)
    73330   (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
    log (P/mmHg) = 6.90334 – 1080.996/(234.67 + t/°C); temp range –35 to 84°C (Antoine eq. for liquid state,
        Dreisbach 1959)
    73300   (interpolated-Antoine eq., temp range –18 .477 to 55.36°C, Zwolinski & Wilhoit 1971)
    73340*   (derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 6.88564 – 1071.578/(233.513 + t/°C); temp range –18 .477 to 55.36°C (Antoine eq., Zwolinski
        & Wilhoit 1971)
    73000, 78380 (calculated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.05468 – 1095.41/(236.322 + t/°C); temp range –58 to –38.2°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    log (P/kPa) = 6.05329 – 1092.997/(236.002 + t/°C); temp range –16 to 33°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)

73350 (interpolated-Antoine eq., temp range –52 to –24°C, Dean 1985, 1992)

$\log (P/mmHg) = 7.01187 – 1126.159/(238.88 + t/°C)$; temp range –52 to –24°C (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.88564 – 1071.518/(233.51 + t/°C)$; temp range –19 to 55°C (Antoine eq., Dean 1985, 1992)

73350 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.13677 – 1126,159/(–34.266 + T/K)$; temp range 221–254 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.01–54 – 1071.578/(–39.637 + T/K)$; temp range 254–316 K (Antoine eq.-II, Stephenson & Malanowski 1987)

73330, 10770 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

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

7840 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

6230, 6520 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

7780 (calculated-P/C, Mackay & Shiu 1981)

14940 (calculated-MCI χ, Nirmalakhandan & Speece 1988)

7780 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.05 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

1.91 (calculated-molar volume V_M, Wang et al. 1992)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

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

$k_{O3} = 16.5 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)

$k_{O3}* = 1.25 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} for the reaction with ozone in air at 296 K, measured range 278–323 K (static system-chemiluminescence, Atkinson et al. 1982)

$k_{OH}* = (9.26 \pm 1.5) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 299 K, measured range 299–422 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982)

$k_{OH} = 10.1 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 297 ± K, k_{OH}(calc) = 9.40×10^{-11} cm^3 molecule^{-1} s^{-1} (relative rate method, Ohta 1983)

$k_{O3}* = (0.58 – 1.25) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} between 260–296 K (Atkinson & Carter 1984)

$k_{O3} = 1.4 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 0.8 d^{-1}, $k_{OH} = 9.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 8 d^{-1}, and $k_{NO3} = 5.8 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 12 d^{-1} (Atkinson & Carter 1984)

$k_{NO3} = (3.23 \pm 0.38) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 295 ± 1 K (relative rate method, Atkinson et al. 1984a)

$k_{NO2} = (10.3 \pm 0.3) \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with NO$_2$ at 295 ± 2 K (relative rate method, Atkinson et al. 1984b)

$k_{O3} = 1.2 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}, $k_{OH} = 9.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 3.2 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1984b)

$k_{OH} = 10.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = 9.98 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, 9.26×10^{-11} cm^3 molecule^{-1} s^{-1} at 299 K (Atkinson 1985)

$k_{OH} = (101 \pm 2) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 23.7 ± 0.5°C (Edney et al. 1986)

$k_{NO3} = 1.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Benter & Schindler 1988)

$k_{OH}* = 1.01 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 1.01 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 1.43 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

$k_{OH} = 5.91 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.01 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

$k_{NO3}* = 6.78 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

$k_{OH}* = 1.01 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3}* = 6.78 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, $k_{O3}* = 12.8 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 3.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated atmospheric lifetimes: 32 h due to reaction with O$_3$ in 24-h period, 2.9 h with OH radical during daytime, and 3.6 h for NO$_3$ radical during nighttime for "clean atmosphere"; 10 h for reaction with O$_3$ in 24-h period, 1.4 h with OH radical during daytime, and 22 min with NO$_3$ radical during nighttime in "moderately polluted atmosphere" (Atkinson et al.1984a, Winer et al. 1984);

atmospheric lifetimes are calculated to be 28.3 h for the reaction with O$_3$, 2.9 h with OH radicals and 0.083 h with NO$_3$ radicals, all based on the reaction rate constants with O$_3$, OH and NO$_3$ radicals in the gas phase (Atkinson & Carter 1984)

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant of 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.2.2.1
Reported aqueous solubilities of 2-methyl-1,3-butadiene (isoprene) at various temperatures

| Pavlova et al. 1966		Shaw 1989a		Góral et al. 2004	
shake flask-GC		IUPAC tentative values		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
20	544.8	20	540	20	530
40	664.6	25	610	25	530
50	760.9	40	660	40	530
60	867.1	50	760		
		60	870		
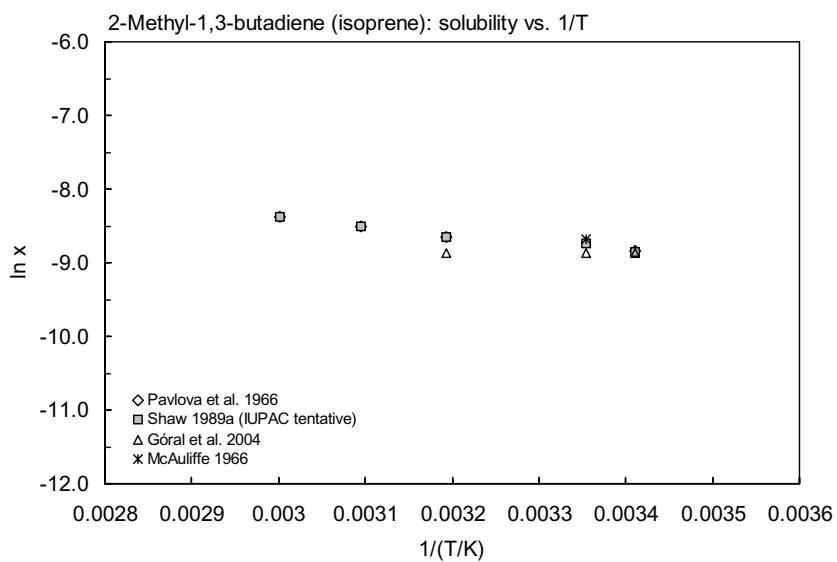
FIGURE 2.1.2.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-1,3-butadiene.

TABLE 2.1.2.2.2
Reported vapor pressures of 2-methyl-1,3-butadiene (isoprene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A[1 - \Phi/(T/K)]$	(5) where $\log A = a + bT + cT^2$		

1.

Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
							liquid
−79.8	133.3	16.836	53718	−57.598	842.86	−51.561	1333
−62.3	666.6	22.506	66816	−55.186	1017	−41.587	2666
−53.3	1333	28.061	83780	−52.77	1221	−35.413	4000
−43.5	2666	33.006	97665	−50.35	1460	−30.714	5333
−32.6	5333	33.469	99260	−47.93	1738	−26.917	6666
−25.4	7999	33.903	100757	−45.507	2060	−23.710	7999
−16.0	13332	34.399	102484	−43.083	2432		liquid
−1.2	26664	34.834	104030	−40.656	2860	−18.447	10666
15.4	53329			−38.227	3349	−14.181	13332
32.6	101325	Antoine eq.				−5.98	19998
		eq. 2	P/mmHg	Cox eq.		0.221	26664
mp/°C	−146.7	A	6.90335	eq. 5	P/atm	5.268	33331
		B	1080.996	Φ	307.217	9.557	39997
		C	234.668	a	0.820543	16.646	53329

TABLE 2.1.2.2.2.2 (*Continued*)

Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				$-b \times 10^{-4}$	8.31178	22.437	66661
		bp/°C	34.067	$c \times 10^{-7}$	10.32622	27.371	79993
						31.693	93326
						32.499	95992
						33.287	98659
						34.059	101325
						bp/°C	34.059
						eq. 2	P/mmHg
						A	6.88654
						B	1071.578
						C	233.513
						for temp range −18–55°C	
						$\Delta H_V/(kJ\ mol^{-1})$ =	
						at 25°C	26.44
						at bp	26.07

2.

Boublikova 1972 (thesis)

in Boublik et al. 1984

t/°C	P/Pa
−16.204	12046
−12.508	14549
−8.291	17921
−4.649	21314
−0.541	25780
2.793	29923
6.725	35493
10.416	41470
14.852	49704
20.211	61295
26.339	77125
33.257	98578
bp/°C	34.036
eq. 2	P/kPa
A	6.05329
B	1092.997
C	236.002
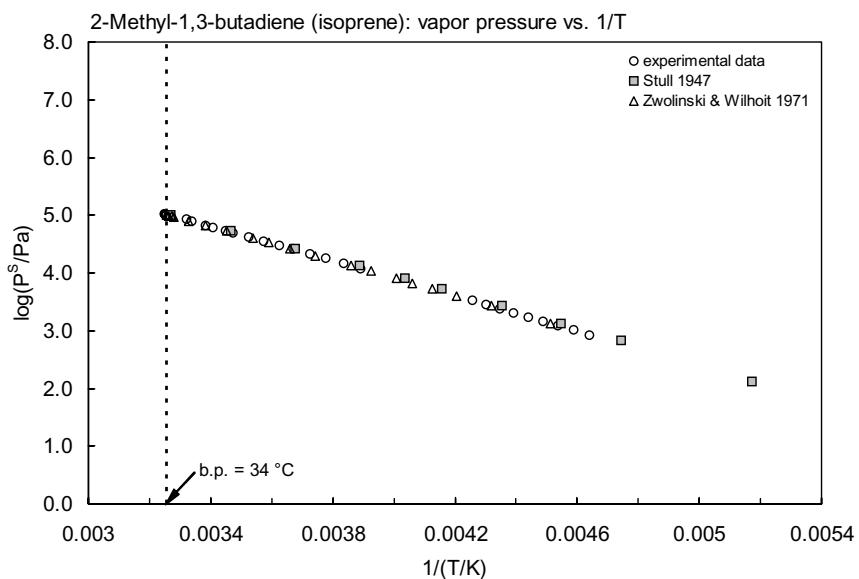
FIGURE 2.1.2.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1,3-butadiene.

2.1.2.2.3   2,3-Dimethyl-1,3-butadiene

Common Name: 2,3-Dimethyl-1,3-butadiene
Synonym:
Chemical Name: 2,3-dimethyl-1,3-butadiene
CAS Registry No: 513-81-5
Molecular Formula: C_6H_{10}; $CH_2 = (CH_3)C(CH_3)=CH_2$
Molecular Weight: 82.143
Melting Point (°C):
     –76   (Lide 2003)
Boiling Point (°C):
     68.8   (Lide 2003)
Density (g/cm³ at 20°C):
   0.7267, 0.7222   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
     113.0, 113.7 (20°C, 25°C, calculated-density)
     125.8   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
     327   (quoted, Hine & Mookerjee 1975)
     226   (calculated-fragment solubility constants, Wakita et al. 1986)
     94.3, 226   (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
     19200   (calculated-Antoine eq., Dreisbach 1959)
     log (P/mmHg) = 7.02388 – 1220.88/(225.9 + t/°C); temp range –6 to 116°C (Antoine eq. for liquid state, Dreisbach 1959)
     20160   (interpolated-Antoine eq., Boublik et al. 1984)
     log (P/kPa) = 6.25005 – 1302.766/(238.42 + t/°C); temp range 0.04–68.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
     20160   (interpolated-Antoine eq., Dean 1985, 1992)
     log (P/mmHg) = 7.1197 – 1299.69/(238.09 + t/°C); temp range 0–68.5°C (Antoine eq., Dean 1985, 1992)
     20150   (interpolated-Stephenson & Malanowski 1987)
     log (P_L/kPa) = 6.3266 – 1346.0/(–30.15 + T/K); temp range 273–342 K (Antoine eq., Stephenson & Malanowski 1987)
     log (P/mmHg) = 29.9755 – 2.5677 × 10³/(T/K) –7.8544·log (T/K) + 2.2361 × 10⁻¹⁰·(T/K) + 2.4591 × 10⁻⁶·(T/K)²; temp range 197–526 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C) :
     4830   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
     5420, 6990 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
     21100   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:

   Volatilization:

   Photolysis:

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

   k_{OH} = $(1.25 \pm 0.05) \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K; k_{OH}(calc) = 1.26×10^{-10} cm^3 $molecule^{-1}$ s^{-1} (relative rate method, Ohta 1983)

   k_{OH} = 1.22×10^{-10} cm^3 $molecule^{-1}$ s^{-1} at 297 K (Atkinson 1985, 1989)

   k_{NO3} = 2.3×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Benter & Shindler 1988)

   k_{OH} = 1.22×10^{-10} cm^3 $molecule^{-1}$ s^{-1}, k_{NO3} = 1.052×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Sabljic & Güsten 1990)

   k_{NO3} = 2.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1991)

   k_{OH} = 1.22×10^{-10} cm^3 $molecule^{-1}$ s^{-1}, k_{NO3} = 2.1×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, and k_{O3}* = 26.5×10^{-18} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1997)

   Hydrolysis:

   Biodegradation:

   Biotransformation:

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

Half-Lives in the Environment:

   Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2}$ = 19 h, based on rate constant k = 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.2.4   1,4-Pentadiene

Common Name: 1,4-Pentadiene
Synonym:
Chemical Name: 1,4-pentadiene
CAS Registry No: 591-93-5
Molecular Formula: C_5H_8; $CH_2=CHCH_2CH=CH_2$
Molecular Weight: 68.118
Melting Point (°C):
   –148.2   (Lide 2003)
Boiling Point (°C):
   26   (Lide 2003)
Density (g/cm³ at 20°C):
   0.6608, 0.6557   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
   103.1, 103.9 (20°C, 25°C, calculated-density)
   103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   6.14   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   49.41, 52/3 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   558   (shake flask-GC, McAuliffe 1966)

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.):
   105100*   (interpolated-Antoine eq. regression, temp range –83.5 to 26.1°C, Stull 1947)
   63774*   (20.669°C, ebulliometry, measured range 14.7–26.7°C (Forziati et al. 1950)
   log (P/mmHg) = 6.84880 – 1025.016/(232.354 + t/°C); temp range 14.7–26.7°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
   97900   (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
   log (P/mmHg) = 6.84880 – 1025.016/(232.354 + t/°C); temp range –41 to 72°C (Antoine eq. for liquid state, Dreisbach 1959)
   3611*   (–43.083°C, inclined-piston manometer, measured range –60.01 to –43.083°C, Osborn & Douslin 1969)
   98000   (interpolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)
   97940*   (derived from compiled data, temp range –57.16 to 26°C, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.83543 – 1017.995/(231.461 + t/°C); temp range –33.271 to 46.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = [–0.2185 × 6826.6/(T/K)] + 7.899113; temp range –83.5 to 26.1°C (Antoine eq., Weast 1972–73)
   98300, 99400 (extrapolated-Antoine equations, Boublik et al. 1984)
   log (P/kPa) = 6.06018 – 1063.485/(236.447 + t/°C); temp range –78.84 to –18.08°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   log (P/kPa) = 6.34694 – 1239.949/(238.278 + t/°C); temp range –60.0 to –26.05°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   97930   (interpolated-Antoine eq., Dean 1985, 1992)
   log (P/mmHg) = 7.17401 – 1155.378/(244.30 + t/°C); temp range –57 to –37°C (Antoine eq., Dean 1985, 1992)
   log (P/mmHg) = 6.83543 – 1017.995/(231.46 + t/°C); temp range –33 to 47°C (Antoine eq., Dean 1985, 1992)
   97900   (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.29891 - 1155.378/(-28.852 + T/K)$; temp range 216–234 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.96033 - 1017.995/(-41.698 + T/K)$; temp range 236–307 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 23.7408 - 2.0505 \times 10^3/(T/K) - 5.679 \cdot \log (T/K) - 5.9671 \times 10^{-11} \cdot (T/K) + 1.1242 \times 10^{-6} \cdot (T/K)^2$; temp range 125–479 K (vapor pressure eq., Yaws 1994)

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

12140	(calculated1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
15640	(calculated-bond contribution, Hine & Mookerjee 1975)
12000	(calculated-P/C, Mackay & Shiu 1981)
13620	(calculated-MCI χ, Nirmalakhandan & Speece 1988)
11946	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

2.48	(shake flask, Log P Database, Hansch & Leo 1987)
2.48	(recommended, Sangster 1989)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

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

$k_{OH} = (50.6 \pm 1.3) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K; k_{OH}(calc) = 50.2 × 10⁻¹⁰ cm³ molecule⁻¹ s⁻¹ (relative rate method, Ohta 1983)

$k_{OH} = 5.33 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 297 K (Atkinson 1985, Atkinson 1989)

$k_{OH} = 5.1 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at room temp (Atkinson et al. 1984b)

$k_{NO3} = 7.8 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 298 K (fast flow system, Benter & Shindler 1988)

$k_{OH} = 5.3 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant k = 1.0 × 10⁷ M⁻¹ s⁻¹ for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.2.4.1

Reported vapor pressures of 1,4-pentadiene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A[1 - \Phi /(T/K)]$	(5) where $\log A = a + bT + cT^2$		

Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–83.5	133.3	14.706	66811	–60.01	1071.4	–57.162	1333
–66.2	666.6	20.699	83774	–57.598	1291	–47.57	2666
–57.1	1333	24.931	97660	–55.186	1550	–41.49	4000
–47.7	2666	25.384	99253	–52.77	1851	–36.492	5333
–37.0	5333	25.806	100752	–50.35	2201	–33.271	6666
–30.0	7999	26.287	102480	–47.93	2605	–30.168	7999
–20.0	13332	26.714	104026	–45.507	3072	–25.069	10666
–6.70	26664			–43.083	3611	–20.933	13332
8.30	53329	bp/°C	25.967			–12.976	19998
26.1	101325					–6.956	26664
		Antoine eq.		Cox eq.		–2.053	33331
mp/°C		eq. 2	P/mmHg	eq. 5	P/atm	2.115	39997
		A	6.84880	Φ	299.117	9.009	53329
		B	1025.016	a	0.812446	14.642	66661
		C	232.354	–b × 10^{-4}	7.52279	19.445	79993
				c × 10^{-7}	8.34048	23.654	93326
						24.439	95992
						25.206	98659
						25.958	101325

eq. for temp–33–46.7°C:

|	
eq. 2	P/mmHg
A	6.83543
B	1017.995
C	231.461
bp/°C	25.958
$\Delta H_v/(kJ\ mol^{-1}) =$	
at 25°C	25.15
at bp	25.15
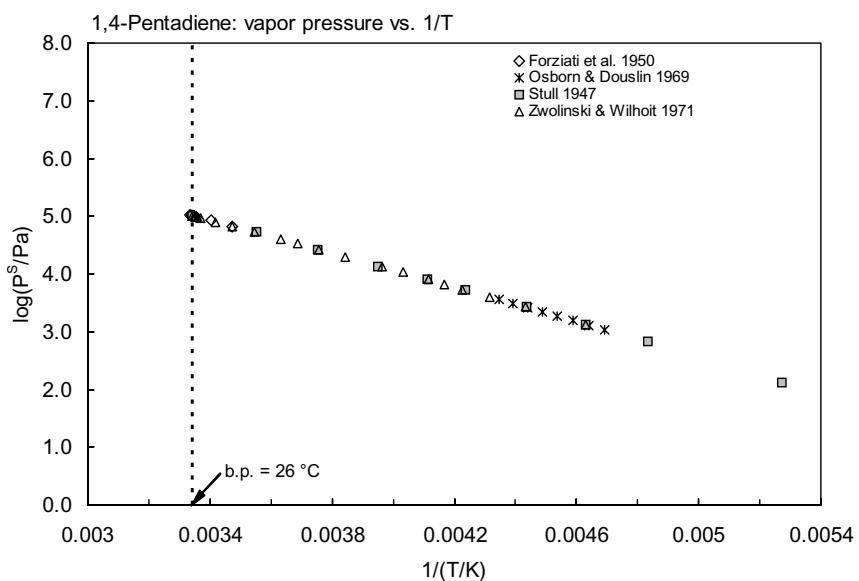
FIGURE 2.1.2.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-pentadiene.

2.1.2.2.5   1,5-Hexadiene
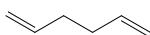
Common Name: 1,5-Hexadiene
Synonym:
Chemical Name: 1,5-Hexadiene
CAS Registry No: 592-42-7
Molecular Formula: C_6H_{10}; $CH_2=CH(CH_2)_2CH=CH_2$
Molecular Weight: 82.143
Melting Point (°C):
    –140.7   (Lide 2003)
Boiling Point (°C):
    59.4   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6920   (Weast 1984)
    0.6923, 0.6878   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    119.0   (20°C, calculated-density, Wang et al. 1992)
    125.8   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    169   (shake flask-GC, McAuliffe 1966)
    320   (14°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    27730   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 7.00740 – 1184.99/(227.7 + t/°C); temp range –13 to 102°C (Antoine eq. for liquid state, Dreisbach 1959)
    32077*   (26.95°C, static method-Hg manometer, measured range 26.95–46.13°C, Letcher & Marsicano 1974)
    29690   (interpolated-Antoine eq., Dean 1985, 1992)
    log (P/mmHg) = 6.5741 – 1013.5/(214.8 + t/°C); temp range 0–59°C (Antoine eq., Dean 1985, 1992)
    29670, 29690   (interpolated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.7368 – 1032.0/(–56.15 + T/K); temp range 273–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.98314 – 1159.908/(–40.998 + T/K); temp range 299–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = 10.5886 – 2.0106 × 10³/(T/K) + 0.28813·log (T/K) – 9.562 × 10⁻³·(T/K) + 7.164 × 10⁻⁶·(T/K)²; temp range 132–507 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    13620   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    17550, 23130   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    17150   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
    2.40   (calculated-π substituent constant, Hansch et al. 1968)
    2.29   (calculated-MCI χ, Murray et al. 1975)
    2.45   (calculated-fragment const., Yalkowsky & Morozowich 1980)
    2.68   (calculated-hydrophobicity const., Iwase et al. 1985)

2.80   (recommended, Sangster 1989)
2.8208   (calculated-UNIFAC group contribution, Chen et al. 1993)
2.78   (calculated-f const., Müller & Klein 1992)
2.43   (calculated-molar volume V_M, Wang et al. 1992)
2.75   (recommended, Sangster 1993)
2.73   (selected, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:
    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:
        $k_{OH} = 6.16 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 297 ± 2 K (relative rate method, Ohta 1983)
        $k_{OH} = 6.35 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, 5.85×10^{-11} cm^3 molecule^{-1} s^{-1} with 1,3-butadiene and propylene as
            standard substances respectively at 297 ± 2 K (relative rate method, Ohta 1983)
        $k_{OH} = 6.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
    Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
    Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and
        $t_{1/2}$ = 19 h, based on rate constant of 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes by singlet oxygen in aquatic
        system (Mill & Mabey 1985).

TABLE 2.1.2.2.5.1
Reported vapor pressures of 1,5-hexadiene at various temperatures

Letcher & Marsicano 1974

static method-Hg manometer

t/°C	P/Pa
26.95	32077
28.93	34690
31.62	38530
34.54	43036
36.94	47169
39.96	52622
41.77	56022
43.04	58622
46.13	65221

Antoine eq.
log P = A – B/(C + T/K)

|	P/mmHg
A	6.6228
B	1037.35
C	–55.52
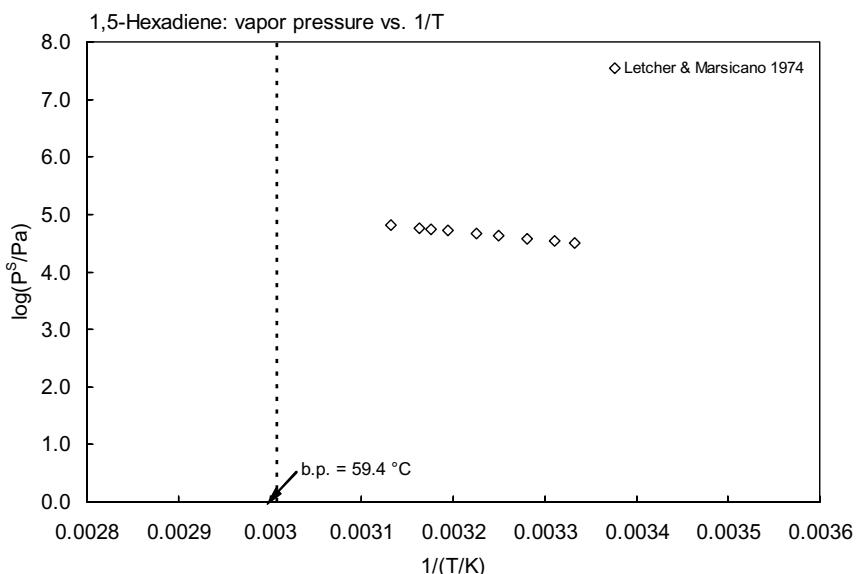
FIGURE 2.1.2.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 1,5-hexadiene.

2.1.2.2.6   1,6-Heptadiene
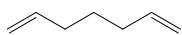
Common Name: 1,6-Heptadiene
Synonym:
Chemical Name: 1,6-heptadiene
CAS Registry No: 3070-53-9
Molecular Formula: C_7C_{12}
Molecular Weight: 96.170
Melting Point (°C):
    –129   (Lide 2003)
Boiling Point (°C):
    90   (Lide 2003)
Density (g/cm³ at 20°C): 0.714
Molar Volume (cm³/mol):
    134.0   (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992)
    148.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    44.0   (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
    2.90   (calculated-π substituent constants, Hansch et al. 1968)
    2.73   (calculated-MCI χ, Murray et al. 1975)
    3.31   (calculated-fragment const., Müller & Klein 1992)
    2.85   (calculated-molar volume V_M, Wang et al. 1992)
    3.2189   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant and Half-Lives:

Half-Lives in the Environment:
    Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2}$ = 19 h, based on rate constant of 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.3   Alkynes

2.1.2.3.1   1-Butyne

Common Name: 1-Butyne
Synonym: ethyl acetylene, but-1-yne
Chemical Name: 1-butyne
CAS Registry No: 107-00-6
Molecular Formula: C_4H_6, $CH_3CH_2C{\equiv}CH$
Molecular Weight: 54.091
Melting Point (°C):
     –125.7   (Lide 2003)
Boiling Point (°C):
     8.08   (Lide 2003)
Density (g/cm³ at 20°C):
     0.650. 0.65 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
     83.22   (20°C, calculated-density)
     81.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     6.03   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     40.9, 36.9   (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
     2870   (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
     log (P/mmHg) = 6.97497 – 986.46/(232.85 + t/°C); temp range –67 to 43°C (Antoine eq. for liquid state, Dreisbach 1959)
     188251   (derived from compiled data, Zwolinski & Wilhoit 1971)
     log (P/mmHg) = 7.07338 – 1101.71/(235.81 + t/°C); temp range –30.8 to 26.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
     log (P/mmHg) = [–0.2185 × 6596.9/(T/K)] + 8.032581; temp range –92.5 to 8.7°C (Antoine eq., Weast 1972–73)
     log (P/mmHg) = 6.98198 – 988.75/(233.01 + t/°C); temp range –68 to 27°C (Antoine eq., Dean 1985, 1992)
     188220   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
     log (P_L/kPa) = 6.10688 – 988.75/(–40.14 + T/K); temp range 205–289 K (Antoine eq., Stephenson & Malanowski 1987)
     log (P/mmHg) = 43.8278 – 2.4255 × 10³/(T/K) –14.141·log (T/K) + 8.2138 × 10⁻³·(T/K) + 7.4889 × 10⁻¹⁴·(T/K)²; temp range 147–443 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
     1880   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
     2210, 1800   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
     1910   (calculated-P/C, Mackay & Shiu 1981)
     2820   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
     1846   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
     1.44, 1.48   (quoted, calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: 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:
        $k_{O3} = 1.79 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 298 K (static system-IR, Dillemuth et al. 1963)
        $k_{O3} = (33 \pm 5) \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 294 ± 1 K (static system-UV, DeMore 1971)
        $k_{O3} = (19.7 \pm 2.6) \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 294 ± 2 K (relative rate method, Atkinson et al.1984b)
        $k_{OH}* = (10.42 \pm 1.38) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K, measured range 253–343 K (discharge flow-
            resonance fluorescence, Boodaghians et al. 1987)
        $k_{OH} = 8.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
        $k_{OH} = 8.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} cm^3 molecule^{-1} s^{-1}, $k_{O3} = 2.0 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} at 298 K
            (Atkinson 1990)
        $k_{O3} = 1.79 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 298 K; and 1.79×10^{-20} cm^3 molecule^{-1} s^{-1}, 4.0×10^{-21} cm^3 molecule^{-1}
            s^{-1} at 294 K (literature review, Atkinson 1991)
   Hydrolysis:
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.2.3.2   1-Pentyne
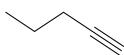
Common Name: 1-Pentyne
Synonym: pent-1-yne
Chemical Name: 1-pentyne
CAS Registry No: 627-19-0
Molecular Formula: C_5H_8; $CH{\equiv}C(CH_2)_2CH_3$
Molecular Weight: 68.118
Melting Point (°C):
    –90   (Lide 2003)
Boiling Point (°C):
    40.1   (Lide 2003)
Density (g/cm³ at 20°C):
    0.6901, 0.6849 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    98.71, 99.46 (20°C, 25°C, calculated-density)
    103.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    1570   (shake flask-GC, McAuliffe 1966)
    1049   (generator column-GC, Tewari et al. 1982a,b)
    1363   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    57520   (calculated from determined data, Dreisbach 1959)
    log (P/mmHg) = 6.97263 – 1095.42/(227.53 + t/°C); temp range –50 to 70°C (Antoine eq. for liquid state, Dreisbach 1959)
    57600   (interpolated-Antoine eq., temp range –33 to 61°C Zwolinski & Wilhoit 1971)
    57462   (derived from compiled data, Zwolinski & Wilhoit 1971)
    log (P/mmHg) = 7.04614 – 1092.52/(227.18 + t/°C); temp range –33 to 61°C (Antoine eq., Zwolinski & Wilhoit 1971)
    57540   (interpolated-Antoine eq., temp range –44 to 61°C, Dean 1985)
    log (P/mmHg) = 6.96734 – 1092.52/(227.18 + t/°C); temp range –44 to 61°C (Antoine eq., Dean 1985, 1992)
    57540   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.09224 – 1092.52/(–45.97 + T/K); temp range 229–315 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 33.8369 – 2.4684 × 10³/(T/K) – 9.4301·log (T/K) + 6.1345 × 10⁻¹⁰·(T/K) + 4.676 × 10⁻⁶·(T/K)²; temp range 167–481 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    2536   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    2980, 2660 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    2500   (calculated-P/C, Mackay & Shiu 1981)
    3422   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
    4983   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    1.98   (shake flask-UV, Hansch et al. 1968, Hansch & Anderson 1967)
    2.12   (generator column-GC, Tewari et al. 1982a,b)

1.98   (recommended, Sangster 1989, 1993)

1.98   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

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

        k_{OH}* = $(11.17 \pm 0.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987, quoted, Atkinson 1989)

        k_{NO3} = 7.54×10^{-16} cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1991)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

2.1.2.3.3   1-Hexyne
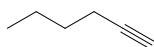
Common Name: 1-Hexyne
Synonym: hex-1-yne
Chemical Name: 1-hexyne
CAS Registry No: 693-02-7
Molecular Formula: C_6H_{10}; $C_4H_9C{\equiv}CH$
Molecular Weight: 82.143
Melting Point (°C):
     –131.9   (Dreisbach 1959; Lide 2003)
Boiling Point (°C):
     71.33   (Dreisbach 1959)
     71.3   (Lide 2003)
Density (g/cm³ at 20°C):
     0.7155, 0.7155   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
     114.8   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
     125.8   (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, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
     360   (shake flask-GC, McAuliffe 1966)
     686   (generator column-GC, Tewari et al. 1982a,b)
     688   (generator column-GC, Miller et al. 1985)
     392   (calculated-recommended liquid–liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C):
     18140   (calculated-Antoine eq., Dreisbach 1959)
     log (P/mmHg) = 6.91212 – 1194.6/(225.0 + t/°C); temp range –8 to 118°C (Antoine eq. for liquid state, Dreisbach
          1959)
     18145   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
     log (P$_L$/kPa) = 6.03702– 1194.6/(–48.15 + T/K); temp range 265–391 K (Antoine eq., Stephenson & Malanowski
          1987)
     log (P/mmHg) = 55.7231 – 3.2541 × 10³/(T/K) –18.405·log (T/K) + 9.5814 × 10^{-3}·(T/K) + 9.2278 × 10^{-14}·(T/K)²;
          temp range 141–516 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol):
     4020   (calculated-1/K$_{AW}$, C$_W$/C$_A$, reported as exptl., Hine & Mookerjee 1975)
     4210, 4020   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
     4310   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
     2166   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K$_{OW}$:
     2.48   (calculated-π substituent constants, Hansch et al. 1968)
     2.73   (generator column-GC, Tewari et al. 1982a,b)
     2.73   (recommended, Sangster 1989, 1993)
     2.73   (selected, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, 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 and/or the Arrhenius expression see reference:

        k_{OH}* = $(12.6 \pm 0.04) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987; quoted, Atkinson 1989)

        k_{NO_3} = 1.60×10^{-15} cm^3 molecule^{-1} s^{-1} at 295 K (Atkinson 1991)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

2.1.2.3.4   1-Heptyne
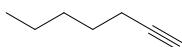
Common Name: 1-Heptyne
Synonym:
Chemical Name: 1-heptyne
CAS Registry No: 628-71-7
Molecular Formula: C_7H_{12}
Molecular Weight: 96.170
Melting Point (°C):
    –81   (Lide 2003)
Boiling Point (°C):
    99.7   (Lide 2003)
Density (g/cm³ at 20°C):
    0.7330   (Weast 1984)
    0.7328, 0.7283   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    131.2   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
    148.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    94.0   (shake flask-GC, McAuliffe 1966)
    107   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    7000   (Antoine eq., Dreisbach 1959)
    4298   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.27249 – 1314.492/(208.097 + t/°C); temp range 63.1–99.98°C (Antoine eq. from reported exptl.
        data, Boublik et al. 1984)
    7500   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.4039 – 1392.4/(–56.55 + T/K); temp range 336–373 K (Antoine eq., Stephenson & Malanowski
        1987)
    log (P/mmHg) = 38.1255 – 3.064 × 10³/(T/K) – 10.679·log (T/K) + 1.2244 × 10⁻¹⁰·(T/K) + 3.668 × 10⁻⁶·(T/K)²;
        temp range 154–537 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):
    6830   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    5950, 6090 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    5420   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
    7160   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    2.98   (calculated-π substituent constants, Hansch et al. 1968)
    2.93   (calculated-MCI χ, Murray et al. 1975)
    2.98   (calculated-molar volume V_M, Wang et al. 1992)
    2.99   (calculated-fragment const., Müller & Klein 1992)
    3.18   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

2.1.2.3.5   1-Octyne
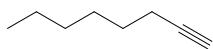
Common Name: 1-Octyne
Synonym:
Chemical Name: 1-octyne
CAS Registry No: 629-05-0
Molecular Formula: C_8H_{14}; $C_6H_{13}C{\equiv}CH$
Molecular Weight: 110.197
Melting Point (°C):
    –79.3   (Dreisbach 1959; Lide 2003)
Boiling Point (°C): 127–128
    126.3   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.7461, 0.7419   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm^3/mol):
    147.7   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
    170.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    24.0   (shake flask-GC, McAuliffe 1966)
    25.4   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    1813   (calculated-Antoine eq., Dreisbach 1959)
    log (P/mmHg) = 7.02447 – 1413.8/(215.0 + t/°C); temp range 25–170°C (Antoine eq. for liquid state, Dreisbach 1959)
    1723   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.36895 – 1997.558/(202.608 + t/°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    1715   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.19321 – 1427.434/(–214.625 + T/K); temp range 84.8–126.26 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
    8208   (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    8208, 9000 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    6827   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
    8325   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    3.48   (calculated-π substituent constants, Hansch et al. 1968)
    3.37   (calculated-MCI χ, Murray et al. 1975)
    3.49   (calculated-molar volume V_M, Wang et al. 1992)
    3.52   (calculated-f const., Müller & Klein 1992)
    3.84   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

2.1.2.3.6   1-Nonyne
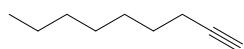
Common Name: 1-Nonyne
Synonym:
Chemical Name: 1-nonyne
CAS Registry No: 3452-09-3
Molecular Formula: C_9H_{16}; $C_7H_{15}C \equiv CH$
Molecular Weight: 124.223
Melting Point (°C):
    –50   (Dreisbach 1959; Lide 2003)
Boiling Point (°C): 150–151
    150.8   (Dreisbach 1959; Lide 2003)
Density (g/cm³ at 20°C):
    0.7570   (Weast 1984)
    0.7568, 0.7527   (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
    164.1   (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)
    192.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    7.20   (shake flask-GC, McAuliffe 1966)
    6.30   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C):
    835   (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
    log (P/mmHg) = 6.77410 – 1404.7/(210.0 + t/°C); temp range 50–223°C (Antoine eq. for liquid state, Dreisbach
        1959)

Henry's Law Constant (Pa m³/mol):
    14600   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    11600, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    8700   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
    14400   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
    3.98   (calculated-π substituent constants, Hansch et al. 1968)
    3.81   (calculated-MCI χ, Murray et al. 1975)
    3.98   (calculated-molar volume V_M, Wang et al. 1992)
    4.05   (calculated-fragment const., Müller & Klein 1992)
    4.50   (calculated-UNIFAC group contribution, Chen et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

2.1.2.4 Cycloalkenes

2.1.2.4.1 Cyclopentene

Common Name: Cyclopentene
Synonym:
Chemical Name: cyclopentene
CAS Registry No: 142-29-0
Molecular Formula: C_5H_8
Molecular Weight: 68.118
Melting Point (°C):
 –135.0 (Lide 2003)
Boiling Point (°C):
 44.2 (Lide 2003)
Density (g/cm³ at 20°C):
 0.7720, 0.7665 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
 88.2 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
 92.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 27.92, 26.96 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 0.48, 3.36; 3.84(–186.08, –135.05°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
 29.83, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
 535 (shake flask-GC, McAuliffe 1966)
 611 (shake flask-titration with bromine, Natarajan & Venkatachalam 1972)
 1645 (shake flask-GC, Pierotti & Liabastre 1972)
 540 (suggested "tentative" value, IUPAC Solubility Data Series, Shaw 1989a)
 719 (calculated-liquid-recommended liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
 39890* (19.77°C, static method-quartz spiral gauge, measured range –42.75 to 19.77°C, Lister 1941)
 43375* (21.028°C, ebulliometry, measured range 11.3–45.024°C, Forziati et al. 1950)
 $\log (P/mmHg) = 6.92066 – 1121.818/(233.446 + t/°C)$; temp range 11.3–45.0°C (Antoine eq., ebulliometry, Forziati et al. 1950)
 50690 (calculated by formula, Dreisbach 1955)
 $\log (P/mmHg) = 6.92066 – 1121.818/(233.446 + t/°C)$; temp range –30 to 105°C (Antoine eq. for liquid state, Dreisbach 1955)
 $\log (P/atm) = [1– 317.520/(T/K)] \times 10^{\{0.814441 – 7.42372 \times 10^{-4} \cdot (T/K) + 8.49035 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 223.2–393.2 K (Cox eq., Chao et al. 1983)
 $\log (P/mmHg) = 6.92066 – 1121.818/(223.45 + t/°C)$; temp range not specified (Antoine eq., Dean 1985, 1992)
 50710 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/kPa) = 6.01617 – 1105.926/(–41.615 + T/K)$; temp range 249–318 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/mmHg) = 30.1132 – 2.3537 \times 10^3/(T/K) –8.0609 \cdot \log (T/K) – 5.7786 \times 10^{-11} \cdot (T/K) + 3.4591 \times 10^{-6} \cdot (T/K)^2$; temp range 138–507 K (vapor pressure eq., Yaws 1994)

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

  6370   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
  3580, 9650 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
  6460   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
  2957, 3408, 3863, 4372* (10, 15, 20, 25°C, headspace-GC, measured range 10–25°C, Bakierowska & Trzeszczyñski 2003)
  ln $(1/K_{AW})$ = 6.989 – 1915/(T/K); temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyñski 2003

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

  1.75   (calculated-π substituent const., Hansch et al. 1968)
  1.76   (calculated-molar volume V_M, Wang et al. 1992)
  2.25   (calculated-fragment const., Müller & Klein 1992)
  2.1791   (calculated-UNIFAC group contribution, Chen et al. 1993)
  2.80   (calculated-UNIFAC activity coeff., Dallos et al. 1993)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

  Volatilization:
  Photolysis:
  Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O3} with O₃ or as indicated, *data at other temperatures see reference:
    k_{O3} = 8.13 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (Japar et al. 1974; quoted, Adeniji et al. 1981)
    k_{O3} = 9.69 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)
    k_{O3} = (2.75 ± 0.33) × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 297 ± 1 K (Atkinson et al. 1983a)
    k_{OH} = (6.39 ± 0.23) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)
    k_{O3} = 4.97 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 291.5 K in synthetic air (Bennett et al. 1987)
    k_{O3} = (62.4 ± 3.5) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K in a smog chamber (Nolting et al. 1988)
    k_{OH} = 4.99 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 3 K, and k_{OH} = 5.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ relative to propene (relative rate method, Rogers 1989)
    k_{OH} = (5.02 – 6.73) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (literature review, Atkinson 1989)
    k_{OH} = 4.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, k_{NO3} = 4.6 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)
    k_{OH} = 6.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 5.81 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Sabljic & Güsten 1990)
    k_{OH} = 6.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 5.3 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, k_{O3}* = 5.7 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹, and $k_{O(3P)}$ = 2.1 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom, at 298 K (recommended, Atkinson 1997)
  Hydrolysis:
  Biodegradation:
  Biotransformation:
  Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

  Air: photooxidation rate constant of 4.97 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ for the reaction with O₃ in synthetic air was determined at atmospheric pressure at 291.5 K (Bennett et al. 1987);
    rate constant k = 4.99 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with OH radicals in air at 298 K (Rogers 1989).
  Surface water: $t_{1/2}$ ~ 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals in aquatic system, and $t_{1/2}$ = 40 d, based on rate constant k = 2 × 10⁵ M⁻¹ s⁻¹ for the oxidation of cyclic olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.1.1

Reported vapor pressures and Henry's law constants of cyclopentene 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)	
$\log P = A - B/(T/K) - C·\log (T/K) + D·[P/(T/K)^2]$	(5)	
$\log (P/atm) = A'[1- (T_B/T)]$	(6) where $\log A' = a + bT + cT^2$	

Vapor pressure				Henry's law constant	
Lister 1941		**Forziati et al. 1950**		**Bakierowska & Trzeszczyñski 2003**	
static-quartz spiral gauge		ebulliometry		headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	Pa m³ mol⁻¹
–42.75	1447	11.325	28994	10	2957
–24.18	4742	15.718	34940	15	3408
0	17292	21.028	43375	20	3863
19.77	39890	26.506	53710	25	4372
		32.34	66807		
		39.678	93760	$\ln (1/K_{AW}) = 6.989 - 1915/(T/K)$	
		43.146	97653		
		43.624	99247		
		44.071	100744		
		44.576	102469		
		45.024	104009		
		bp/°C	44.242		
		Antoine eq.			
		eq. 2	P/mmHg		
		A	6.92066		
		B	1121.818		
		C	233.446		
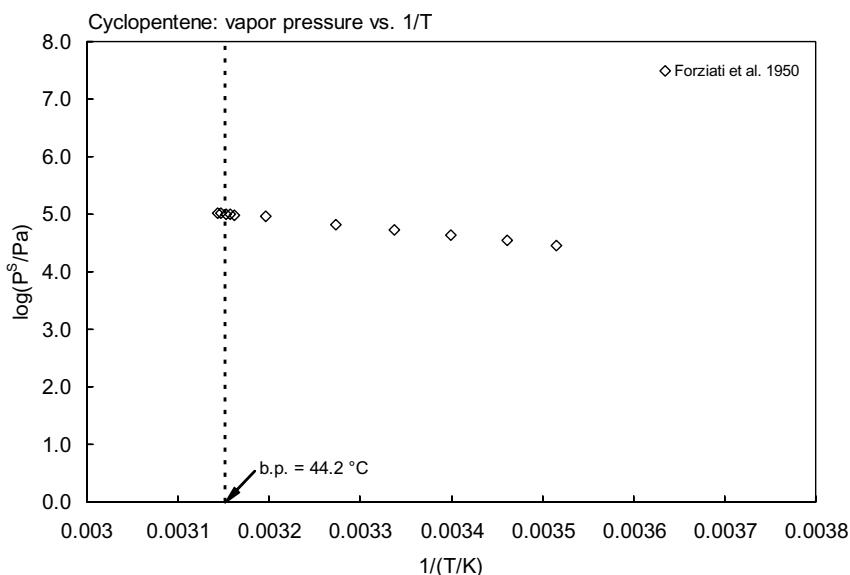
FIGURE 2.1.2.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for cyclopentene.

2.1.2.4.2   *Cyclohexene*

Common Name: Cyclohexene
Synonym: 1,2,3,4-tetrahydrobenzene, tetrahydrobenzene
Chemical Name: cyclohexene
CAS Registry No: 110-83-8
Molecular Formula: C_6H_{10}
Molecular Weight: 82.143
Melting Point (°C):
    –103.5   (Weast 1982–83; Lide 2003)
Boiling Point (°C):
    82.98   (Lide 2003)
Density (g/cm^3 at 20°C):
    0.8110, 0.8061 (20°C, 25°C, Dreisbach 1959)
    0.8102   (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
    101.4   (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
    110.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    33.142, 30.485 (25°C, bp, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    29.125, 27.276 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    3.28   (Riddick et al. 1986)
    4.23, 3.28; 7.51(–134.45, –104.45°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    49.85, 41.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional
    data at other temperatures designated * are compiled at the end of this section.):
    130   (shake flask-cloud point, McBain & Lissant 1951)
    160   (Farkas 1964)
    213   (shake flask-GC, McAuliffe 1966)
    299*   (25.11°C, shake flask-GC, measured 5.11–45.21°C, Pierotti & Liabastre 1972)
    281, 286   (23.5°C, elution chromatography, Schwarz 1980)
    160   (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
    246*   (calculated-liquid-liquid equilibrium LLE data, temp range 278.2–318.2 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section.):
    160, 752, 3345, 8723* (–44.42, –24.85, 0. 18.45°C, static method-quartz spiral gauge, Lister 1941)
    11734*   (24.794°C, ebulliometry, measured range 12.2–83.9°C Forziati et al. 1950)
    log (P/mmHg) = 6.888617 – 1229.973/(224.104 + t/°C); temp range 12.2–83.9°C (Antoine eq., ebulliometry
        measurements, Forziati et al. 1950)
    11840   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 6.88617 – 1229.973/(224.104 + t/°C); temp range 3.0–146°C (Antoine eq. for liquid state,
        Dreisbach 1955)
    19885*   (36.875°C, comparative ebulliometry, measured range 36.875–91.378°C, Meyer & Hotz 1973)
    log (P/mmHg) = [1– 356.172/(T/K)] × 10^{0.873674 – 9.73841 × 10^{-4}·(T/K) + 10.9078 × 10^{-7}·(T/K)^2}; temp
        range 213.2–364.53 K (Cox eq., Chao et al. 1983)

11800 (selected lit., Riddick et al. 1986)

log (P/kPa) = 7.109 – 2289.0/(T/K); temp range: not specified (Antoine eq., Riddick et al. 1986)

11850 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.997323 – 1221,899/(–49.978 + T/K); temp range 309–385 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 52.1749 – 3.238 × 10³/(T/K) – 16.878·log (T/K) + 8.0388 × 10⁻³·(T/K) + 1.3259 × 10⁻¹³·(T/K)²; temp range 170–560 K (vapor pressure eq., Yaws 1994)

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

4020 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

4946, 13310 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

4568 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

3960 (23°C, batch air stripping-IR, Nielsen et al. 1994)

2069, 2467, 2618, 2965 (10, 15, 20, 25°C, headspace-GC, Bakierowska & Trzeszçzyñski 2003)

ln (1/K_{AW}) = 5.860 – 1691/(T/K); temp range 10–25°C, headspace-GC, Bakierowska & Trzeszçzyñski 2003)

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

2.16 (calculated-π substituent constants, Hansch et al. 1968)

2.86 (shake flask-GC, Leo et al. 1975)

1.90 (shake flask-GC, Canton & Wegman 1983)

2.86 (recommended, Sangster 1989, 1993)

2.86 (recommended, Hansch et al. 1995)

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

2.92* (20.29°C, from GC-determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

$k_{O(3P)}$ = 2.20 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom (Herron & Huie 1973)

k_{OH} = 6.77 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Atkinson et al. 1979)

k_{O3} = 1.69 × 10⁻¹⁶ cm³ molecule⁻¹ at 298 K (Japar et al. 1974)

k_{O3} = 2.04 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)

k_{O3} = (1.04 ± 0.14) × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 297 ± 1 K (Atkinson et al. 1983a)

k_{OH} = (6.43 ± 0.17) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)

k_{OH} = (64.1 ± 2.5) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K (relative rate method, Ohta 1983)

k_{O3} = 1.04 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 297 K (Atkinson & Carter 1984)

k_{O3} = 1.04 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹, k_{OH} = 6.4 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 0.29 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, $k_{O(3P)}$ = 21 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with O(³P) atom and k_{NO2} < 0.2 × 10⁻²⁰ cm³ molecule⁻¹ s⁻¹ with NO₂ (Atkinson & Aschmann 1984)

k_{O3} = 1.51 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ in synthetic air at 295 K (Bennett et al. 1987)

k_{O3} = (7.8 ± 0.5) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

k_{OH} = 5.40 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K and k_{OH} = 6.1 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ relative to propene (relative rate method, Rogers 1989)

k_{OH} = 6.77 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

k_{OH} = 6.77 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 5.3 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)

k_{OH} = 6.75 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 5.3 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Sabljic & Güsten 1990)

$k_{NO3} = 5.28 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 295 K (quoted, Atkinson 1991)

$k_{OH} = 6.77 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3}* = 5.9 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, and $k_{O3}* = 81.4 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 2.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO$_2$ radicals in aquatic system, and $t_{1/2} = 40$ d, based on rate constant k = 2×10^5 M^{-1} s^{-1} for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.2.1
Reported aqueous solubilities of cyclohexene at various temperatures

| Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004	
shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
5.11	280	5	–	5.1	265
15.21	298.5	15	–	15.2	251
25.11	299	20	–	20	246
35.21	302.5	25	160	23.5	246
45.21	310.5	35	–	25	246
		45	–	25.1	246
				35.2	251
				45.2	265
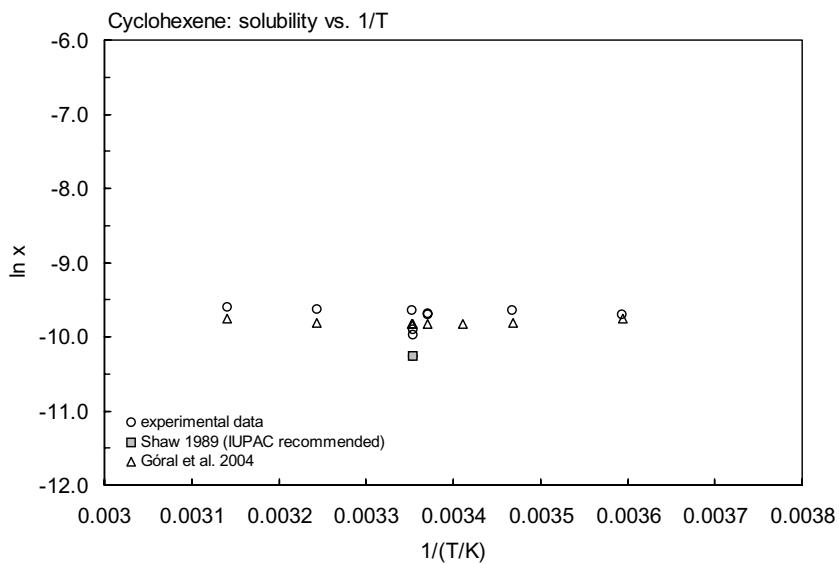
FIGURE 2.1.2.4.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for cyclohexene.

TABLE 2.1.2.4.2.2

Reported vapor pressures and octanol-air partition coefficients of cyclohexene at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot [P/(T/K)^2]$ (5)

$\log (P/atm) = A'[1 - (T_B/T)]$ (6) where $\log A' = a + bT + cT^2$

| Vapor pressure						log K_OA	
Lister 1941		**Forziati et al. 1950**		**Meyer & Hotz 1973**		**Gruber et al. 1997**	
static-quartz spiral gauge		ebulliometry		comparative ebulliometry		GC det'd activity coeff.	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–44.42	160	12.236	6417	36.875	19885	20.29	2.926
–24.85	752	15.920	7709	43.560	26084	30.3	2.762
0	3345	19.137	9006	49.795	33189	40.4	2.594
18.45	8723	22.063	10344	55.785	41404	50.28	2.447
		24.794	11734	62.537	52551		
$\Delta H_V/(kJ\ mol^{-1}) = 32.59$		28.490	13858	68.815	64943		
	at 27°C	32.702	16651	75.354	80213		
		36.996	19958	81.075	95764		
		40.976	23358	86.112	111325		
		46.302	28995	91.378	129633		
		51.191	35060				
		57.107	43376	bp/°C	82.945		
		63.200	53712				
		69.708	66808	Antoine eq.			
		76.766	83761	eq. 3	P/cmHg		
		81.757	97648	A	5.872420		
		82.292	99248	B	1221.899		
		82.791	100746	C	223.1720		
		83.353	102470				
		83.852	104010	Cox eq.			
				eq. 6	P/atm		
		eq. 2	P/mmHg	a	0.833958		
		A	6.88617	–b × 10³	0.742586		
		B	1229.973	c × 10⁶	0.767278		
		C	224.104	T_B/K	356.0954		
		bp/°C	82.979				
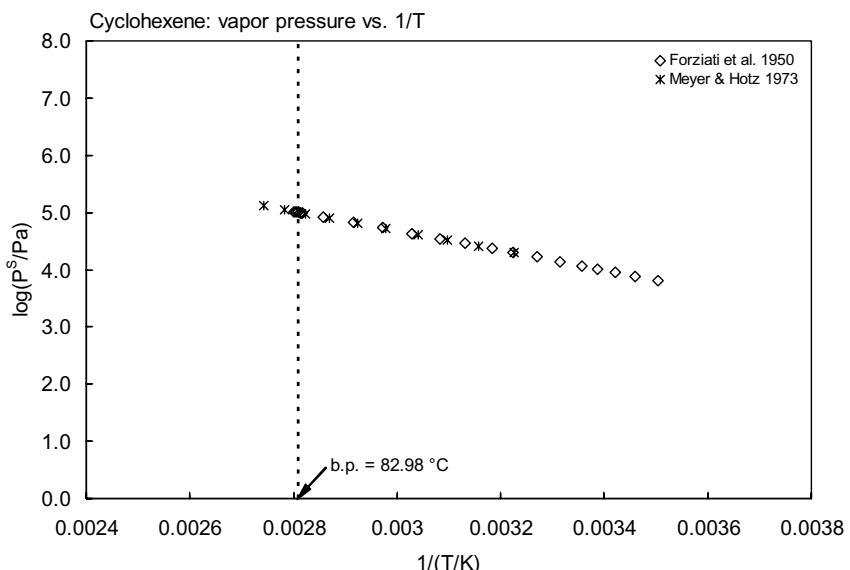
FIGURE 2.1.2.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexene.
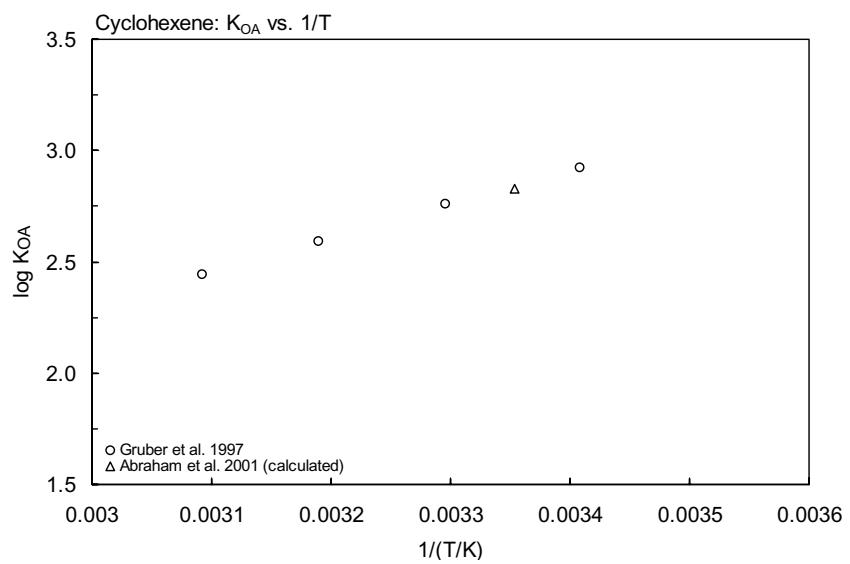

FIGURE 2.1.2.4.2.3 Logarithm of K_{OA} versus reciprocal temperature for cyclohexene.

2.1.2.4.3 1-Methylcyclohexene
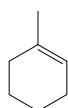
Common Name: 1-Methylcyclohexene
Synonym:
Chemical Name: 1-methylcyclohexene
CAS Registry No: 591-49-1
Molecular Formula: C_7H_{12}
Molecular Weight: 96.170
Melting Point (°C):
    –120.4   (Lide 2003)
Boiling Point (°C):
    110.3   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8102, 0.8058 (20°C, 25°C, Dreisbach 1959; Weast 1982–83)
Molar Volume (cm³/mol):
    118.7   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
    133.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    37.75, 32.70 (25°, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    6.63   (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    43.16, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    52.0   (shake flask-GC, McAuliffe 1966)
    64.1   (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    4080   (calculated by formula, Dreisbach 1955)
    $\log (P/\text{mmHg}) = 6.86861 - 1308.0/(218.0 + t/°C)$; temp range 25–165°C, (Antoine eq. for liquid state, Dreisbach 1955)
    3933   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    $\log (P_L/\text{kPa}) = 6.0101 - 1311.087/(-56.045 + T/K)$; temp range 333–384 K (Antoine eq., Stephenson & Malanowski 1987)
    4858   (25.25°C, transpiration method, Verevkin et al. 2000)
    $\ln (P/\text{Pa}) = 23.65 - 4531/(T/K)$; temp range 275.4–313.4 K (transpiration method, Verevkin et al. 2000)

Henry's Law Constant (Pa m³/mol at 25°C):
    7660   (calculated-$1/K_{AW}$, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
    7485, 14260 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
    11070   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
    1.05   (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
    2.20   (calculated-molar volume V_M, Wang et al. 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

     Volatilization:

     Photolysis:

     Oxidation: 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:

         $k_{OH} = 9.44 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 305 K (Darnall et al. 1976, Atkinson 1989)

         $k_{NO3} = (2.87 \pm 0.34) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 295 K (relative rate method, Atkinson et al. 1984a)

         $k_{NO2} < 0.20 \times 10^{-20}$ cm³ molecule⁻¹ s⁻¹; $k_{O3} = 1.4 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹; $k_{OH} = 6.4 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹; $k_{NO3} = 2.9 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹; and $k_{O(3P)} = 2.1 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ with O(³P) atom at room temp. (relative rate method, Atkinson et al. 1984b)

         $k_{OH} = 9.45 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 294 K (Atkinson 1985)

         $k_{OH} = 9.4 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1990)

         $k_{OH} = 9.4 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{NO3}* = 1.7 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{O3} = 1.65 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹, and $k_{O(3P)} = 9.0 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom, at 298 K (recommended, Atkinson 1997)

     Hydrolysis:

     Biodegradation:

     Biotransformation:

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

Half-Lives in the Environment:

     Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals in aquatic system, and $t_{1/2} = 40$ d, based on rate constant $k = 2 \times 10^5$ M⁻¹ s⁻¹ for the oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.4.4   Cycloheptene

Common Name: Cycloheptene
Synonym: suberene
Chemical Name: cycloheptene
CAS Registry No: 628-92-2
Molecular Formula: C_7H_{12}
Molecular Weight: 96.170
Melting Point (°C):
    –56   (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
    115   (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
    0.8228   (Weast 1982–83)
Molar Volume (cm³/mol):
    116.9   (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
    129.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    36.73   (27°C, Lister 1941)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    5.28, 0.71, 0.97; 6.96 (–119.15, –63.15, –56.15°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    42.14, 45.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    66.0   (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    188, 821, 2636, 6547 (–21.44, 0, 19.82, 39.06°C, static method-quartz spiral gauge, Lister 1941)
    2670   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    log $(P_L/kPa) = 7.27243 – 2011.9/(T/K)$; temp range 251–313 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
    2.57   (calculated-π substituent constants, Hansch et al. 1968)
    2.75   (calculated-MCI χ, Murray et al. 1975)
    3.073   (calculated-UNIFAC group contribution, Chen et al. 1993)
    2.58   (calculated-molar volume V_M, Wang et al. 1992)
    3.37   (calculated-fragment const., Müller & Klein 1992)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: 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} = $(3.19 \pm 0.36) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 297 ± 1 K (Atkinson et al. 1983a; quoted, Atkinson & Carter 1984)

k_{OH} = $(7.08 \pm 0.11) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (relative rate method, Atkinson et al. 1983b)

k_{OH} = 7.44×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al. 1983b, Atkinson 1989)

k_{O3} = $(28.3 \pm 1.5) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

k_{NO3} = 2.80×10^{-13} cm^3 molecule^{-1} s^{-1}, k_{OH} = 7.13×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

k_{NO3} = 4.84×10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1991)

k_{OH} = 7.4×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 4.8×10^{-13} cm^3 molecule^{-1} s^{-1}, and k_{O3}* = 2.45×10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2}$ ~ 320 h and 9×10^4 d for oxidation by OH and RO$_2$ radicals in aquatic system, and $t_{1/2}$ = 40 d, based on rate constant k = 2×10^5 M^{-1} s^{-1} for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.4.5   Cyclooctene

Common Name: Cyclooctene
Synonym:
Chemical Name: cyclooctene
CAS Registry No: 931-87-3 (*cis*-octene), 931-89-5 (*trans*-octene)
Molecular Formula: C_8H_{14}
Molecular Weight: 110.197
Melting Point (°C):
    –12, –59   (*cis*-, *trans*-cyclooctene, Weast 1982–83; Lide 2003)
    –14.5 to –15.5   (*cis*-cyclooctene, Stephenson & Malanowski 1987)
Boiling Point (°C):
    138, 143   (*cis*-, *trans*-cyclooctene, Weast 1982–83; Lide 2003)
Density (g/cm³):
    0.8472, 0.8483   (20°C, *cis*-, *trans*-cyclooctene, Weast 1982–83)
Molar Volume (cm³/mol):
    130.1   (*cis*-, 20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
    129.9   (*trans*-, 20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
    146.7   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.57   (27°C, Lister 1941)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
    22.9*   (generator column-GC/FID, measured range 273.15–313.15 K, Dohányosová et al. 2004)
    $\ln x = -33.3561 + 20.8640/\tau + 43.2804 \cdot \ln \tau$, $\tau = [(T/K)/298.15]$, temp range 273.15–313.15 K (generator column-GC/FID, Dohányosová et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    209.3, 774.6, 2333, 5948 (0, 19.83, 40.36, 60.22°C, static method-quartz spiral manometer, Lister 1941)
    $\log (P_L/\text{kPa}) = 7.3641 - 2194.3/(T/K)$, temp range 273–441 K (*cis*-cyclooctene, Antoine eq., Stephenson & Malanowski 1987)
    1010   (interpolated from data of Lister 1941, temp range 273.15–313.15 K, Dohányosová et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C. Additional data at other temperatures designated * are compiled at the end of this section.):
    4842*   (derived from measured mole fraction solubility and solute fugacity, temp range 273.15–313.15 K, Dohányosová et al. 2004)

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

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

    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_{O_3}* = 3.75 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (*cis*-cyclooctene, recommended, Atkinson 1997)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

TABLE 2.1.2.4.5.1
Reorted aqueous solubilities and Henry's law constants of cyclooctene at various temperatures

| Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC/FID		smoothed raw exptl data		from solute fugacity f and x	
T/K	S/g·m^{-3}	T/K	S/g·m^{-3}	T/K	H/(Pa m^3/mol)
	raw data				
274.15	20.39	273.15	19.9	273.15	1184.4
274.15	20.14	278.15	20.2	278.15	1625.4
278.15	20.39	283.15	20.7	283.15	2196
278.15	19.59	288.15	21.3	288.15	2898
283.15	21.24	293.15	22.0	293.15	3780
283.15	20.45	298.15	22.9	298.15	4842
288.15	20.94	303.15	23.9	303.15	6120
288.15	20.63	308.15	25.1	308.15	7614
293.15	21.92	313.15	26.5	313.15	9378
298.15	23.63				
298.15	24.61	ln x = A + B/τ + C ln τ			
303.15	22.84		τ = T/298.15		
303.15	23.14	A	−33.3561		
308.15	27.24	B	20.8640		
308.15	24.73	C	23.4396		
308.15	26.88				
313.15	27.31				
313.15	24.80				
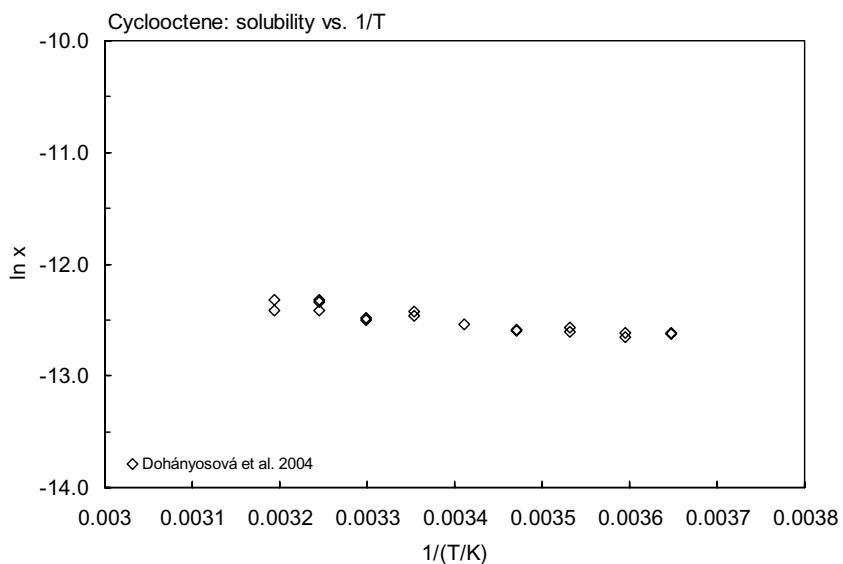
FIGURE 2.1.2.4.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for cyclooctene.
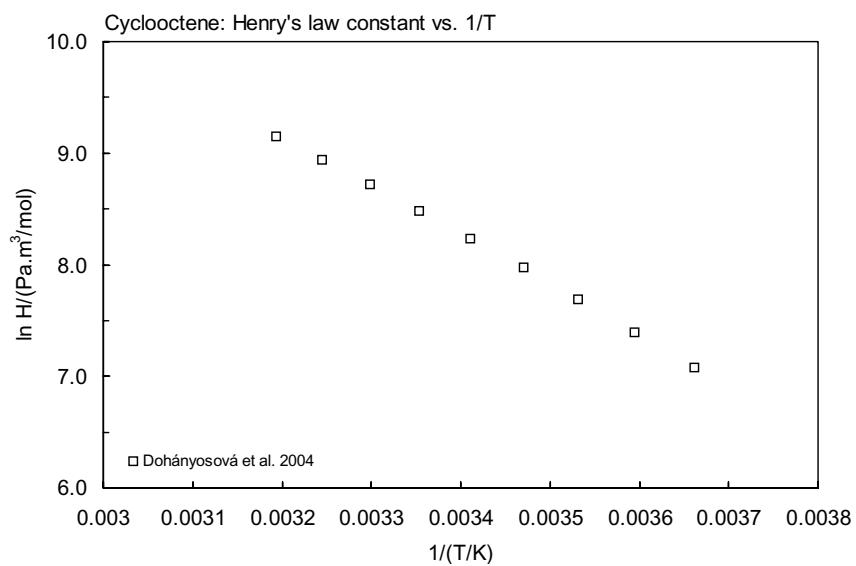

FIGURE 2.1.2.4.5.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctene.

2.1.2.4.6   *1,4-Cyclohexadiene*

Common Name: 1,4-Cyclohexadiene
Synonym: 1,4-dihyrobenzene
Chemical Name: 1,4-cyclohexadiene
CAS Registry No: 628-41-1
Molecular Formula: C_6H_8
Molecular Weight: 80.128
Melting Point (°C):
     –49.2   (Weast 1983–83; Lide 2003)
Boiling Point (°C):
     85.5   (Lide 2003)
Density (g/cm³ at 20°C):
     0.8471   (Weast 1982–83)
Molar Volume (cm³/mol):
     93.60   (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
     103.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
     0.82, 5.72; 6.53 (–81.15, –49.15°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
     29.16, 38.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
     compiled at the end of this section.):
     700   (shake flask-GC, McAuliffe 1966)
     930*   (shake flask-GC, measured range 5.11–45.21°C, Pierotti & Liabstre 1972)
     800*   (recommended, temp range 5–45°C, IUPAC Solubility Data Series, Shaw 1989a)
     979*   (calculated-liquid-liquid equilibrium LLE data, temp range 278.3–318.4 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
     temperatures designated * are compiled at the end of this section.):
     11892*   (31.1°C, static method-Hg manometer, measured range 304.25–322.23 K, Letcher & Marsicano
         1974)
     $\log (P/\text{mmHg}) = [1 - 368.566/(T/K)] \times 10^{\{0.916704 - 6.81678 \times 10^{-4} \cdot (T/K) - 7.02362 \times 10^{-7} \cdot (T/K)^2\}}$; temp
         range 304.25–322.23 K (Cox eq., Chao et al. 1983)
     8973   (extrapolated-Antoine eq., Boublik et al. 1984)
     $\log (P/\text{kPa}) = 5.86553 - 1176.707/(214.528 + t/°C)$; temp range 31.1–49.08°C (Antoine eq. from reported exptl.
         data, Boublik et al. 1984)
     9009   (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
     $\log (P_L/\text{kPa}) = 6.41736 - 1475.149/(-26.108 + T/K)$; temp range: 304–360 K (Antoine eq., Stephenson &
         Malanowski 1987)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$
     2.30   (shake flask, Log P Database, Hansch & Leo 1987)
     2.48   (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
     2.30   (recommended, Sangster 1989, 1993)
     2.30   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

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

      $k_{O3} = (0.639 \pm 0.074) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 297 ± 1 K (Atkinson et al. 1983a)

      $k_{OH} = (9.48 \pm 0.39) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)

      $k_{NO3} = (2.89 \pm 0.035) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 295 K (Atkinson et al. 1984a)

      $k_{O3} = 63.9 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, $k_{OH} = 9.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 0.29 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, and $k_{NO2} < 0.4 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} with NO_2 (Atkinson et al. 1984b)

      k_{OH}(exptl) = 9.90×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = 1.03×10^{-10} cm^3 molecule^{-1} s^{-1} (Atkinson 1985)

      $k_{NO3} = 7.8 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (fast flow system, Benter & Schindler 1988)

      $k_{OH} = (99.2 - 99.8) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (review, Atkinson 1989)

      $k_{OH} = 9.91 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} and $k_{NO3} = 5.30 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} for the reaction with NO_3 radical at nights (Sabljic & Güsten 1990)

      $k_{NO3} = 6.6 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

      $k_{OH} = 9.95 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 6.6 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, and $k_{O3}^* = 4.6 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

    Surface water: $t_{1/2} \sim$ 320 h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2}$ = 19 h, based on rate constant k = 1.0×10^7 M^{-1} s^{-1} for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.6.1
Reported aqueous solubilities of 1,4-cyclohexadiene at various temperatures

| Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004		Letcher & Marsicano 1974	
shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data		static method-Hg manometer	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	T/K	S/g·m^{-3}
5.11	851.9	5	900	5.1	1068	304.25	11892
15.21	958.5	15	900	15.2	979	307.67	13826
25.11	936.2	25	800	25.0	979	310.76	15812
35.21	963.4	35	1000	25.1	979	312.92	42655
45.21	1010	45	1000	35.2	979	316.67	20238
				45.2	1068	319.94	22998
						322.23	25251
						Antoine eq.,	P/mmHg
						log P = A – B/(C + T/K)	
						A	7.2687
						B	1461.75
						C	–29.4

FIGURE 2.1.2.4.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,4-cyclohexadiene.

2.1.2.4.7 Cycloheptatriene

Common Name: Cycloheptatriene
Synonym: tropilidene
Chemical Name: 1,3,5-cycloheptatriene
CAS Registry No: 544-25-2
Molecular Formula: C_7H_8
Molecular Weight: 92.139
Melting Point (°C):
   –79.5   (Weast 1982–83; Lide 2003)
Boiling Point (°C):
   117   (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
   0.8875   (Weast 1982–83)
Molar Volume (cm³/mol):
   103.0   (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
   114.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
   2.35, 1.16; 3.51   (–93.15, –75.15°C, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
   21.11, 38.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
   620   (shake flask-GC, McAuliffe 1966)
   669*   (25.11°C, shake flask-GC, measured range 5.11–40.21°C, Pierotti & Liabastre 1972)
   640*   (recommended best value, temp range 5–45°C, IUPAC Solubility Data Series, Shaw 1989)
   563*   (calculated-liquid-liquid equilibrium LLE data, temp range 278.3–318.4 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
   3136*   (ebulliometry, measured range 0–65°C, Finke et al. 1956)
   $\log (P/\text{mmHg}) = 6.97032 – 1374.065/(t/°C + 220.538)$; temp range 0–65°C (Antoine eq., ebulliometry, Finke et al. 1956)
   2825, 3138 (interpolated-Antoine eq-I, II, Stephenson & Malanowski 1987)
   $\log (P_L/\text{kPa}) = 6.09522 – 1374.656/(–52.612 + T/K)$; temp range 273–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   $\log (P_L/\text{kPa}) = 6.12574 – 1390.771/(–53.069 + T/K)$; temp range 273–390 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):
   432   (calculated-P/C from selected data)
   466   (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
   2.63   (shake flask, Eadsforth & Moser 1983)
   3.03   (HPLC-RT correlation, Eadsforth & Moser 1983)
   2.63   (recommended, Sangster 1989)
   2.63   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{\frac{1}{2}}$:
   Volatilization:
   Photolysis:
   Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
      with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
      $k_{O3} = (5.39 \pm 0.078) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}; $k_{OH} = (9.12 \pm 0.23) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for at 294 ± 2
         K (Atkinson et al. 1984b)
      $k_{O3} = 5.39 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} for at 294 K (Atkinson & Carter 1984)
      $k_{OH} = 9.74 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 294 K (Atkinson 1985)
      $k_{NO3} = 1.18 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $k_{OH} = 9.44 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten
         1990)
      $k_{OH} = 96.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 294 K (Atkinson 1989)
      $k_{NO3} = 1.19 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (quoted, Atkinson 1991)
      $k_{OH} = 9.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, and $k_{O3} = 5.4 \times 10^{-17}$ cm^3
         molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
   Hydrolysis:
   Biodegradation:
   Biotransformation:
   Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.2.4.7.1
Reported aqueous solubilities and vapor pressures of cycloheptatriene at various temperatures

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

Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004		Finke et al. 1956	
shake flask-GC		IUPAC recommended		calc-recommended LLE data		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa
5.11	580.9	5	580	5.1	614	0	733.3
10.21	664.5	15	660	15.2	614	15	1815
25.11	669.4	25	640	25.0	563	20	2400
30.21	741.8	35	740	25.1	563	25	3136
40.21	764.8	45	760	35.2	614	30	4058
				45.2	614	35	5198
						40	6591
						45	8286
						50	10327
						55	12774
						60	15672
						65	19094

TABLE 2.1.2.4.7.1 (*Continued*)

Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		**Shaw 1989a**		**Góral et al. 2004**		**Finke et al. 1956**	
shake flask-GC		**IUPAC recommended**		**calc-recommended LLE data**		**ebulliometry**	
t/°C	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**	**t/°C**	**S/g·m⁻³**	**t/°C**	**P/Pa**
						bp/°C	115.60
						$\Delta H_V/(kJ\ mol^{-1}) = 38.70$	
							at 25°C
						eq. 2	P/mmHg
						A	6.97032
						B	1374.656
						C	220.538

Cycloheptatriene: solubility vs. 1/T

◇ Pierotti & Liabastre 1972
▫ Shaw 1989 (IUPAC recommended)
△ Góral et al. 2004
✕ McAuliffe 1966
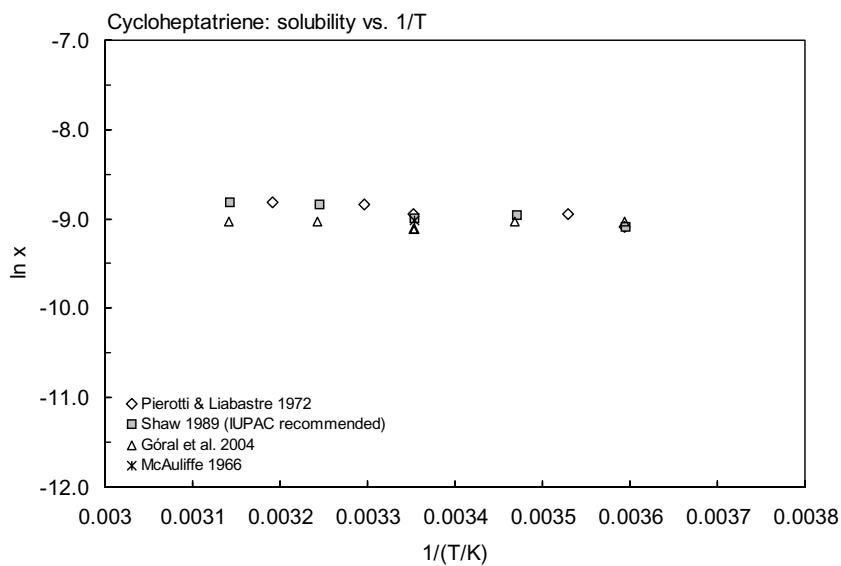
FIGURE 2.1.2.4.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclohepta-triene.
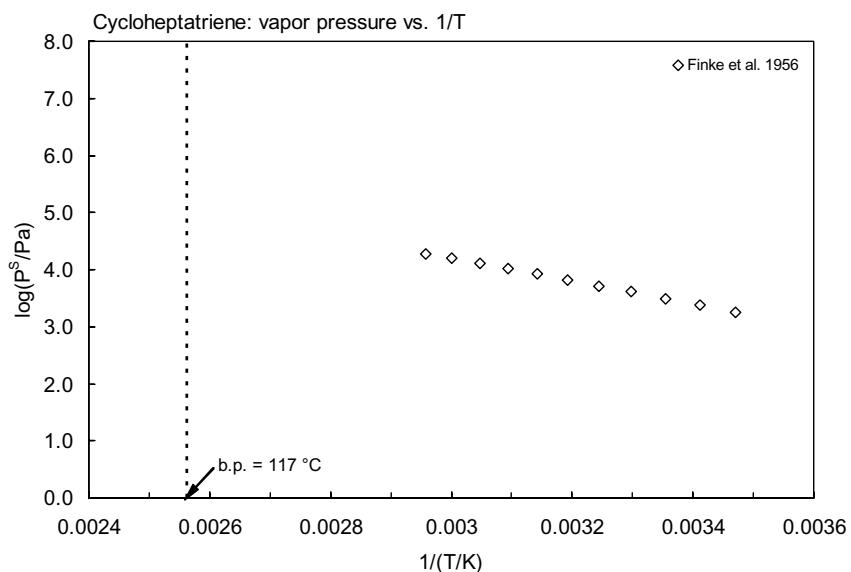
FIGURE 2.1.2.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for cycloheptatriene.

2.1.2.4.8 dextro-*Limonene [(*R*)-(+)-Limonene]*
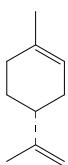
Common Name: *d*-Limonene
Synonym: *d-p*-mentha-1,8,-diene, (R)-(+)-*p*-mentha-1,8-diene, (+)-1-methyl-4-(1-methylethenyl)cyclohexene, *p*-mentha-1,8-diene, carvene, cinene, citrene, cajeputene, kautschin
Chemical Name: *dextro*-limonene, (R)-(+)-limonene
CAS Registry No: 5989-27-5
Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.234
Melting Point (°C):
    –74   (Lide 2003)
Boiling Point (°C):
    178   (Weast 1982–83; Lide 2003)
Density (g/cm³ at 25°C):
    0.8403, 0.8383 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    162.1   (20°C, calculated-density, Stephenson & Malanowski 1987)
    192.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    45.1   (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    13.49   (shake flask-GC, Massaldi & King 1973)
    13.8   (selected lit., Riddick et al. 1986)
    20.44   (shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    275.64   (calculated-Antoine eq. regression, Stull 1947)
    275.5   (interpolated-Antoine eq., Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 10508.4/(T/K)] + 8.016262; temp range 14.0–175°C (Antoine eq., Weast 1972–73)
    2670   (68.2°C, Riddick et al. 1986)
    278, 202   (calculated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.81591 – 2075.62/(–16.65 + T/K); temp range 287–448 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 7.67098 – 2494.342/(T/K); temp range 288–323 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = 9.3771 – 2.8246 × 10³/(T/K) + 1.0584·log (T/K) – 8.9107 × 10⁻³·(T/K) + 4.8462 × 10⁻⁶·(T/K)²; temp range 199–660 K (vapor pressure eq., Yaws 1994)
    213   (activity coefficient-GC, Fichan et al. 1999)

Henry's Law Constant (Pa m³/mol at 25°C):
    2725   (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, log K_{OW}:
    4.38   (RP-HPLC-RT correlation, Griffin et al. 1999)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

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

        $k_{OH} = 9 \times 10^{10}$ cm^3 mol^{-1} s^{-1}, with $t_{1/2} < 0.24$ h (Darnall et al. 1976)

        $k_{OH} = (9.0 \pm 1.35) \times 10^{10}$ M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

        $k_{OH} = 9.0 \times 10^{10}$ M^{-1} s^{-1}, $k_{O3} = 3.9 \times 10^5$ M^{-1} s^{-1}, and $k_{O(3P)} = (6.50 \pm 0.52) \times 10^{10}$ cm^3 M^{-1} s^{-1} for reaction with O(^{3}P) atom at room temp. (Winer et al. 1976)

        k_{OH}(calc) = 13.8×10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = (14.0, 14.2) $\times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1983b)

        $k_{NO3} = (7.7 \pm 1.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 295 K (relative rate technique, Atkinson et al. 1984a)

        $k_{O3} = 6.4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with calculated lifetimes τ = 6 min and 11 min in 24-h in clean and moderately polluted atmosphere, respectively; $k_{OH} = 1.42 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} with calculated $\tau = 2.0$ h and 1.0 h during daytime in clean and moderately polluted atmosphere respectively, $k_{NO3} = 7.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with calculated τ = 9 min and 0.9 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)

        $k_{NO2} < 3.5 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

        $k_{O3} = 6.4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}; $k_{OH} = 1.42 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 7.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $k_{O(3P)} = 1.29 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} with O(^{3}P) atom at room temp. (Atkinson et al. 1984b)

        $k_{O3} = 6.0 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 36 d^{-1}; $k_{OH} = 1.4 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 12 d^{-1}, and $k_{NO3} = 1.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 290 d^{-1} (Atkinson & Carter 1984)

        $k_{O3} = 6.0 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 36 d^{-1}; $k_{OH} = 1.7 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 7.3 d^{-1}, and $k_{NO3} = 1.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 290 d^{-1} at room temp. (Atkinson 1985)

        $k_{OH} = (16.9 \pm 0.5) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 294 ± 1 K (relative rate method, Atkinson et al.1986)

        $k_{O3} = 6.4 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} with calculated τ = 36 min; $k_{OH} = 1.7 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 1.6 h, $k_{NO3} = 1.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 5.0 min for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

        $k_{OH} = (146–171) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 294–305 K (review, Atkinson 1989)

        $k_{OH} = 1.71 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 1.22 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = 2.03 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 7.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom, at 298 K (recommended, Atkinson 1997)

    Hydrolysis:

    Biodegradation:

    Biotransformation:

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

Half-Lives in the Environment:

    Air: $t_{1/2}$ <.24 h in air based on its photooxidation rate constant of 9×10^{13} cm^3 mol^{-1} s^{-1} for the gas phase reaction with hydroxyl radical (Darnall et al. 1976; Lloyd et al. 1976);

        calculated lifetimes: τ =36 min due to reaction with O_3 in 24-h period, τ = 2.0 h with OH radical during daytime, and τ = 9 min for NO_3 radical during nighttime for "clean" atmosphere; τ = 11 min for reaction with O_3 in 24-h period, τ = 1.0 h with OH radical during daytime, and τ = 0.9 min for NO_3 radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a);

        calculated atmospheric lifetimes, τ = 36 min, 1.6 h and 5.0 min for reaction with O_3, OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);

        calculated tropospheric lifetimes τ = 1.1 h, 1.9 h and 53 min due to reactions with OH radical, O_3 and NO_3 radical, respectively, at room temp. (Corchnoy & Atkinson 1990).

2.1.2.4.9   *α-Pinene*
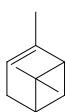
Common Name: α-Pinene
Synonym: *dl*-pinene, 2-pinene
Chemical Name: 2,6,6-trimethylbicyclo[3,1,1]hept-2-ene
CAS Registry No: 7785-70-8
          α-pinene *d*-Form 80-56-8
Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.234
Melting Point (°C):
  –55   (*dl*-Form, Weast 1982–83)
  –64   (*d*-Form, Riddick et al. 1986; Lide 2003)
  –50   (*d*-Form, Stephenson & Malanowski 1987)
Boiling Point (°C):
  156.2   (*dl*-Form, Weast 1982–83; Lide 2003)
  156   (*d*-Form, Stephenson & Malanowski 1987)
  155–156   (*d*-, *l*-Form, Budavari 1989)
Density (g/cm³):
  0.8582   (20°C, *dl*-Form, Weast 1982–83)
  0.8582, 0.8539   (*d*-Form, Riddick et al. 1986)
  0.8592, 0.8591, 0.8590 (20°C, *dl*-, *d*-, *l*-Form, Budavari 1989)
Molar Volume (cm³/mol):
  157.4   (*d*-Form, Stephenson & Malanowski 1987)
  183.7   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  46.61, 39.673   (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

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

  21.8, 3.42; 5.04   (quoted lit. values; shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
  temperatures designated * are compiled at the end of this section.):
  640*, 800   (22.2, 22.5°C, measured range 21.1–148°C, Pickett & Peterson 1929)
  237.3*   (13.25°C, Hg manometer, measured range –6.0 to 13.25°C, Linder 1931)
  666.6*   (24.6°C, summary of literature data, temp range –1.0 to 155.0°C, Stull 1947)
  457*, 655   (21.2, 27.2°C, measured range 19.4–155.75°C, Hawkins & Armstrong 1954)
  678   (interpolated-Antoine eq., Weast 1972–73)
  log (P/mmHg) = [–0.2185 × 9813.6/(T/K)] + 7.898207; temp range –1.0 to 155°C (Antoine eq., Weast 1972–73)
  667   (Verschueren 1983)
  605, 587   (interpolated-Antoine equations, Boublik et al. 1984)
  log (P/kPa) = 6.37971 – 1692.803/(231.558 + t/°C); temp range 21.1–148°C (Antoine eq. from reported exptl.
     data of Pickett & Peterson 1929, Boublik et al. 1984)
  log (P/kPa) = 6.95174 – 1430.936/(206.42 + t/°C); temp range 19.44–155.75°C (Antoine eq. from reported exptl.
     data of Hawkins & Armstrong 1954, Boublik et al. 1984)
  655   (selected, Riddick et al. 1986)
  log (P/kPa) = 25.52644 – 3134.525/(T/K) – 6.16045·log (T/K) (Riddick et al. 1986)

582   (α-pinene *d*-Form, interpolated-Antoine eq., temp range 292–433 K, Stephenson & Malanowski 1987)

log (P/kPa) = 5.92666 – 1414.16/(T/K) (Antoine eq., liquid, temp range 292–433 K (α-pinene *d*-Form, Stephenson & Malanowski 1987)

588   (interpolated-Antoine eq., temp range 19–156°C, Dean 1992)

log (P/mmHg) = 6.8525 – 1446.4/(t/°C + 208.0); temp range 19–156°C (Antoine eq., Dean 1992)

log (P/mbar) = 7.076588 –1511.961/[(T/K) –57.730]; temp range 365–430 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)

log (P/mmHg) = 21.4735 – 2.7156 × 10^3/(T/K) – 5.0076·log (T/K) + 2.8146 × 10^{-3}·(T/K) – 1.5389 × 10^{-6}·(T/K)^2; temp range 209–632 K (vapor pressure eq., Yaws 1994)

613, 581, 465; 529   (quoted lit. values; deduced from exptl. determined activity coeff. at infinite dilution, Fichan et al. 1999)

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

0.194*   (20°C, calculated from measured liquid-phase diffusion coefficients, measured range –10 to 20°C, Zhang et al. 2003)

ln [H'/(M/atm)] = –6.590 + 3800/(T/K); temp range 263–293 K (Zhang et al. 2003)

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

4.44   ((+)-α-pinene, RP-HPLC-RT correlation, Griffin et al. 1999)

4.48   ((–)-α-pinene, RP-HPLC-RT correlation, Griffin et al. 1999)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants k_{O3} for reaction with O_3, k_{OH} with OH radical and k_{NO3} with NO_3 radical at 25°C or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} = (3.48 ± 0.52) × 10^{10} cm^3 M^{-1} s^{-1} at 305 ± 2 K (relative rate method, Winer et al. 1976)

k_{OH} = 3.5 × 10^{10} M^{-1} s^{-1}, k_{O3} = 2.0 × 10^5 M^{-1} s^{-1}, and $k_{O(3P)}$ = (1.60 ± 0.06) × 10^{10} M^{-1} s^{-1} for reaction with O(^{3}P) atom at room temp. (Winer et al. 1976)

k_{OH} = 32 × 10^{-12} cm^3 molecule^{-1} s^{-1}; k_{O3} = 67 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Gaffney & Levine 1979)

k_{O3}* = (8.4 ± 1.9) × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K, measured range 276–324 K, atmospheric lifetime τ = 3–4 h due to reaction with O_3, and τ ~ 4 h due to reaction with OH radical (Atkinson et al. 1982)

k_{OH}* = (6.01 ± 0.82) × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–422 K (flash photolysis-resonance fluorescence, Kleindlenst et al. 1982)

k_{OH}(calc) = 8.7 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs) = (7.6, 5.5, 6.01) × 10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1983b)

k_{OH}* = 60.1 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–422K (Flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)

k_{NO3} = (3.4 ± 0.8) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 ± 1 K (relative rate method, Atkinson et al. 1984a)

k_{O3} = 8.4 × 10^{-17} cm^3 molecule^{-1} s^{-1} with calculated lifetimes of 4.6 h and 1.4 h in 24-h in clean and moderately polluted atmosphere, respectively; k_{OH} = 6.0 × 10^{-11} cm^3 molecule^{-1} s^{-1} with calculated lifetimes of 4.6 h and 2.3 h during daytime in clean and moderately polluted atmosphere, respectively, k_{NO3} = 3.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} with calculated lifetimes of 20 min and 2 min during nighttime in clean and moderately polluted atmosphere respectively at room temp. (Atkinson et al. 1984a)

k_{NO2} < 2.1 × 10^{-20} cm^3 molecule^{-1} s^{-1} for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

$k_{O3} = 8.4 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1}; $k_{OH} = 6.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 3.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $k_{O(3P)} = 640 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} with O(^{3}P) at room temp. (Atkinson et al. 1984b)

$k_{O3} = 8 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 5 d^{-1}; $k_{OH} = 6.0 \times 10^{-12}$ cm^3 molecule^{-1}s^{-1} with a loss rate of 5 d^{-1}, and $k_{NO3} = 6.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with a loss rate of 130 d^{-1} (Atkinson & Carter 1984)

$k_{OH} = (5.45 \pm 0.32) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 294 $\pm$ 1 K (relative rate method, Atkinson et al.1986)

$k_{O3} = 8.4 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} with calculated τ = 5.6 h; $k_{OH} = 5.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 5.1 h, $k_{NO3} = 6.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with τ(calc) = 11 min for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

$k_{O3} = (8.6 \pm 1.3) \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 297 $\pm$ 2 K in a smog chamber (Nolting et al. 1988)

$k_{OH}* = 5.37 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH}* = 5.37 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 5.79 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{O3} = (8.4, 8.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson et al. 1990)

$k_{OH} = 9.12 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} and $k_{NO3} = 5.75 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Müller & Klein 1991)

$k_{OH} = 5.32 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3} = 5.79 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

$k_{NO3}* = 6.16 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1991)

$k_{OH}* = 5.37 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, $k_{NO3}* = 6.16 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, $k_{O3}* = 86.6 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1}, and $k_{O(3P)} = 3.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for the reaction with O(^{3}P) atom, at 298 K (recommended, Atkinson 1997)

k_{OH}(lit.) = 5.45×10^{-11} cm^3 molecule^{-1} s^{-1}; k_{OH}(calc) = 8.5×10^{-11} cm^3 molecule^{-1} s^{-1} (quoted; calculated-QSAR, Peeters et al. 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated lifetimes: τ = 4.6 h due to reaction with O$_3$ in 24-h period, τ = 4.6 h with OH radical during daytime, and τ = 20 min for NO$_3$ radical during nighttime for clean atmosphere; τ = 1.4 h for reaction with O$_3$ in 24-h period, τ = 2.3 h with OH radical during daytime, and τ = 2 min with NO$_3$ radical during nighttime in moderately polluted atmosphere (Atkinson et al.1984a, Winer et al. 1984);

calculated atmospheric lifetimes of 5.6 h, 5.1 h and 11 min for reaction with O$_3$, OH and NO$_3$ radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);

calculated tropospheric lifetimes of 3.4 h, 4.6 h and 2.0 h due to reactions with OH radical, O$_3$ and NO$_3$ radical respectively at room temp. (Corchnoy & Atkinson 1990).

TABLE 2.1.2.4.9.1

Reported vapor pressures of α-pinene at various temperatures and the coefficients for the vapor pressure equations

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

1.

Pickett & Peterson 1929				Linder 1931		Stull 1947	
Ramsay & Young method				Hg manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
21.2	533	134.9	57128	–6.0	54.66	–1.0	133
22.0	573	135.4	57608	1.0	96.0	24.6	666.6
22.2	640	138.5	63728	13.25	237.3	37.3	1333
22.5	800	138.8	64261			51.4	2666

(Continued)

TABLE 2.1.2.4.9.1 (*Continued*)

Pickett & Peterson 1929				Linder 1931		Stull 1947	
Ramsay & Young method				Hg manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
54.7	3040	139.8	65861			66.8	5333
55.3	3200	140.1	66794			76.8	7999
55.5	3306	140.5	67461			90.1	13332
77.4	7839	141.2	68794			110.2	26664
77.5	7906	141.3	69327			132.3	53329
77.7	7959	141.9	70394			155.0	101325
77.9	8026	147.0	80526				
78.6	8253	148.0	83060			mp/°C	−55
79.3	8519						
79.6	8639	bp/°C	155–158				
101.1	19625						
102.8	20758						
103.2	21025						
103.5	21238						
103.7	21371						
103.8	21451						
131.2	52196						
132.3	53462						
132.4	53862						
132.5	53902						
132.7	54089						
132.9	54275						
133.0	54755						
133.1	54862						
133.2	54995						

2.

Hawkins & Armstrong 1954

Hg manometer

t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
19.45	408.0	65.63	4858	95.27	16164	155.77	100601
21.3	457.3	66.54	5121	102.25	20717	155.76	100793
27.25	654.6	68.27	5554	105.9	23430		
29.72	790.6	70.45	6073	106.76	24217	bp/°C	155.9
37.07	1201	75.1	7430	110.53	27438		
46.92	2015	76.04	7698	113.5	30135	eq. 4	P/mmHg
53.69	2832	77.12	8033	115.07	31795	A	26.40174
54.18	2877	79.75	8905	122.11	39478	B	3134.525
56.57	3234	84.71	10859	125.02	42963	C	6.16045
57.09	3309	86.23	11536	129.87	49509	155.77	100601
57.3	3393	88.42	12512	135.72	58678		
62.28	4221	92.01	14299	147.48	80731		
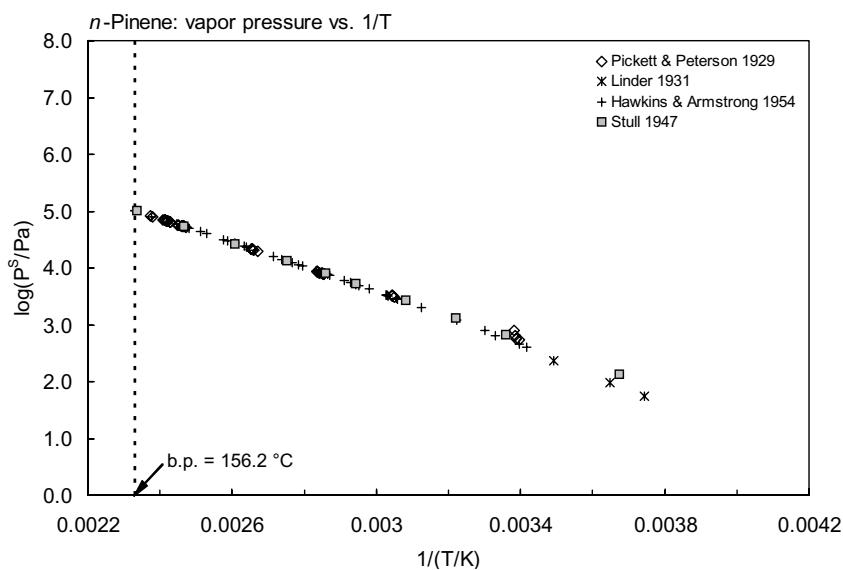
FIGURE 2.1.2.4.9.1 Logarithm of vapor pressure versus reciprocal temperature for α-pinene.

TABLE 2.1.2.4.9.2
Reported Henry's law constants of α-pinene at various temperatures

Zhang et al. 2003

liquid-phase diffusion coefficient

t/°C	H/(Pa m³/mol)
−10	0.0397
0	0.0618
10	0.113
20	0.194

ln (kH/atm) = A − B/(T/K)

eq. 3	H′/(M atm⁻¹)
A	−6.59
B	3800
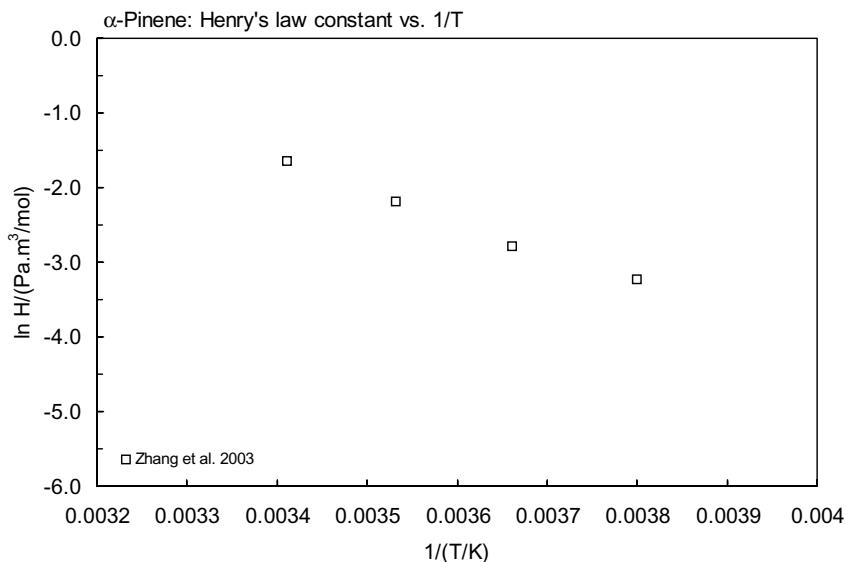
FIGURE 2.1.2.4.9.2 Logarithm of Henry's law constant versus reciprocal temperature for α-pinene.

2.1.2.4.10 β-*Pinene*
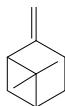
Common Name: β-Pinene
Synonym: β-Pinene *d*, or nopinene; β-Pinene *l*, or 2(10)-pinene
Chemical Name: 6,6-dimethyl-2-methylene bicyclo[3,1,1]heptane
CAS Registry No: 19172-67-3
   β-pinene *l*-Form 127-91-3
Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.234
Melting Point (°C):
 –61.54 (*l*-Form, Riddick et al. 1986)
 –50   (*l*-Form, Stephenson & Malanowski 1987)
 –61.5 (l-Form, Lide 2003)
Boiling Point (°C):
 164–166, 162.4 (*d*-Form, *l*-Form, Weast 1982–83)
 166   (*l*-Form, Riddick et al. 1986; Lide 2003)
 163   (*l*-Form, Stephenson & Malanowski 1987)
 165–166, 164–166, 162–163 (*dl*-, *d*-, *l*-Form, Budavari 1989)
Density (g/cm³):
 0.8654, 0.8694 (20°C, *d*-, *l*-Form, Weast 1982–83)
 0.8667 (25°C, *l*-Form, Riddick et al. 1986)
Molar Volume (cm³/mol):
 157.4 (*l*-Form, Stephenson & Malanowski 1987)
 183.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  43.471, 40.208 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
 32.7, 6.27; 11.04 (quoted lit. values; shake flask-GC, Fichan et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
 temperatures designated * are compiled at the end of this section.):
 613* (Ramsay & Young method, measured range 24.3–158.1°C, Pickett & Peterson 1929)
 666.6* (30.0°C, summary of literature data, temp range 4.2–158.3°C, Stull 1947)
 345*, 447 (23.06, 26.8°C, measured range 18.71–165.91°C, Hawkins & Armstrong 1954)
 501   (interpolated-Antoine eq., Weast 1972–73)
 log (P/mmHg) = [–0.2185 × 10235.8/(T/K)] + 8.633424; temp range 4.2–158.3°C (Antoine eq., Weast 1972–73)
 667   (Verschueren 1983)
 395   (interpolated-Antoine eq., Boublik et al. 1984)
 log (P/kPa) = 6.02052 – 1509.944/(210.05 + t/°C); temp range 18.71–165.9°C (Antoine eq. from reported exptl.
  data of Hawkins & Armstrong 1954, Boublik et al. 1984)
 610   (selected, Riddick et al. 1986)
 log (P/kPa) = 27.90258 – 3318.845/(T/K) – 6.94263·log (T/K) (Riddick et al. 1986)
 391   (*l*-Form, interpolated- Antoine eq., temp range 291–441K, Stephenson & Malanowski 1987)
 log (P/kPa) = 6.04993 – 1520.15/(T/K + 62.75); temp range 291–441 K (*l*-Form, Antoine eq., liquid, Stephenson
  & Malanowski 1987)

394   (interpolated-Antoine eq., Dean 1992)

log (P/mmHg) = 6.8984 – 1511.7/(t/°C + 210.2); temp range 19–156°C (Antoine eq., Dean 1992)

log (P/mbar) = 7.067997 –1539.348/[(T/K) –59.937]; temp range 364–439 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)

log (P/mmHg) = 46.3728 – 3.9789 × 10³/(T/K) –13.284·log (T/K) – 1.3113 × 10⁻¹⁰·(T/K) + 3.4783 × 10⁻⁶·(T/K)²; temp range 120–651 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol):

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

4.16   (RP-HPLC-RT correlation, Griffin et al. 1999)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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

k_{OH} = 42 × 10⁹ L mol⁻¹ s⁻¹, with $t_{1/2}$ = 0.24–2.4 h (Darnall et al. 1976)

k_{OH} = (4.06 ± 0.61) × 10¹⁰ M⁻¹ s⁻¹ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

k_{OH} = 4.1 × 10¹⁰ M⁻¹ s⁻¹; k_{O3} = 2.2 × 10⁴ M⁻¹ s⁻¹; and $k_{O(3P)}$ = (1.51 ± 0.06) × 10¹⁰ M⁻¹ s⁻¹ for reaction with O(³P) atom (Winer et al. 1976)

k_{O3} = 30 × 10⁻¹² cm³ molecule⁻¹ s⁻¹; k_{OH} = 65 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Gaffney & Levine 1979)

k_{O3} = (2.1 ± 0.5) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K with atmospheric lifetime τ ~ 13 h due to reaction with O_3 and τ ~ 4 h due to reaction with OH radical (Atkinson et al. 1982)

k_{OH}* = (7.76 ± 1.1) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 297–423 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)

k_{OH}(calc) = 5.1 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{OH}(obs) = (6.4, 7.76) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ (Atkinson et al. 1983b)

k_{NO3} = (1.4 ± 0.3) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 295 ± 1 K (relative rate method, Atkinson et al. 1984a)

k_{O3} = 2.1 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ with calculated lifetimes τ = 18 h and 5.5 h in 24-h in clean and moderately polluted atmosphere respectively; k_{OH} = 7.8 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ with calculated τ = 3.6 h and 1.8 h during daytime in clean and moderately polluted atmosphere, respectively; k_{NO3} = 1.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with calculated τ = 50 min and 5 min during nightime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)

k_{NO2} = < 2.4 × 10⁻²⁰ cm³ molecule⁻¹ s⁻¹ for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

k_{O3} = 2.1 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹; k_{OH} = 7.8 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 1.4 × 10⁻¹² cm³ molecule⁻¹ s⁻¹; and $k_{O(3P)}$ = 640 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom, at room temp. (Atkinson et al. 1984b)

k_{OH} = (7.95 ± 0.52) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 294 ± 1 K (relative rate method, Atkinson et al.1986)

k_{O3} = 2.1 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ with calculated τ = 18 h; k_{OH} = 8.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ with τ(calc) = 3.5 h, k_{NO3} = 2.5 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with τ(calc) = 28 min for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

k_{NO3} = 2.36 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate method, Atkinson et al. 1988)

k_{O3} = (1.4 ± 0.2) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

k_{OH}* = 7.89 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

k_{OH}* = 7.89 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, k_{NO3} = 2.36 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, and k_{O3} = (2.1; 1.4) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 296 K (Atkinson et al. 1990)

$k_{OH} = 5.62 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹; $k_{NO3} = 2.34 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (Müller & Klein 1991)

$k_{OH} = 7.82 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{NO3} = 2.36 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, at 298K (Sabljic & Güsten 1990)

$k_{NO3} = 2.51 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1991)

$k_{O3} = 12.2 \pm 1.3 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹ at 22 ± 1°C (Grosjean et al. 1993)

$k_{OH}^* = 7.89 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{NO3} = 2.51 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, and $k_{O3}^* = 1.5 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹, and $k_{O(3P)} = 2.7 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for the reaction with O(³P) atom, at 298 K (recommended, Atkinson 1997)

$k_{OH, lit} = 7.95 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹; k_{OH}(calc) $= 6.0 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ (quoted; calculated-QSAR, Peters et al. 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated lifetimes: $\tau = 18$ h due to reaction with O_3 in 24-h period, $\tau = 3.6$ h with OH radical during daytime, and $\tau = 50$ min for NO_3 radical during nighttime for "clean" atmosphere; $\tau = 5.5$ h for reaction with O_3 in 24-h period, $\tau = 1.8$ h with OH radical during daytime, and $\tau = 5$ min with NO_3 radical during nighttime hours in "moderately polluted" atmosphere (Atkinson et al.1984a, Winer et al. 1984);

calculated atmospheric lifetimes of 18 h, 3.5 h and 28 min for reaction with O_3, OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);

calculated tropospheric lifetimes of 2.3 h, 1.1 d and 4.9 h due to reactions with OH radical, O_3 and NO_3 radical respectively at room temp. (Corchnoy & Atkinson 1990).

TABLE 2.1.2.4.10.1

Reported vapor pressures of β-pinene at various temperatures and the coefficients for the vapor pressure equations

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

1.

	Pickett & Peterson 1929					Stull 1947	
	Ramsay & Young method					summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.3	453.3	94.7	13839	131.9	47809	4.2	133.3
24.5	480	95.1	14225	132.1	48329	30.0	666.6
24.7	520	95.7	14585	132.6	48889	42.3	1333
24.8	400	96.0	14705	132.9	49583	58.1	2666
25.0	613	96.2	14905	133.6	50623	71.5	5333
25.4	653	96.5	14905	133.9	50796	81.2	7999
53.5	2486	105.8	20825	154.7	91792	94.0	13332
54.0	2440	106.0	20998	154.9	92126	114.1	26664
54.4	2466	106.4	21305	155.2	92459	136.1	53329
54.6	2520	106.9	21665	156.2	94859	158.3	101325
55.0	2586	107.1	21812	158.0	100258		
68.7	4680	108.2	21932	158.1	100926	mp/°C	–
68.9	4720	131.2	47529				
69.1	4866	131.6	47929	bp/°C	160.2–163.8		
70.9	5240	131.7	47929				

(Continued)

TABLE 2.1.2.4.10.1 (*Continued*)

2.

| Hawkins & Armstrong 1954							
Hg manometer							
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.72	252.0	50.11	1644	81.23	6949	161.22	89634
20.05	284.0	52.32	1812	85.96	8266	165.8	100788
23.09	345.3	56.57	2268	85.86	9983	157.82	101194
26.82	446.6	56.94	2341	90.80	11346		
29.45	517.3	58.86	2550	94.12	12828	bp/°C	166.0
31.68	592.0	59.48	3056	97.33	15948		
32.03	592.0	62.62	3084	103.41	19288	eq. 4	P/mmHg
36.78	793.3	66.52	3534	108.81	24117	A	28.77768
37.09	803.9	68.75	4014	115.50	27972	B	3318.845
39.41	929.3	72.23	4677	125.33	33079	C	6.94243
41.34	1037	75.43	5384	131.39	39762		
45.52	1289	78.59	6141	136.02	45106		
49.41	1580	80.88	6810	149.55	65069		
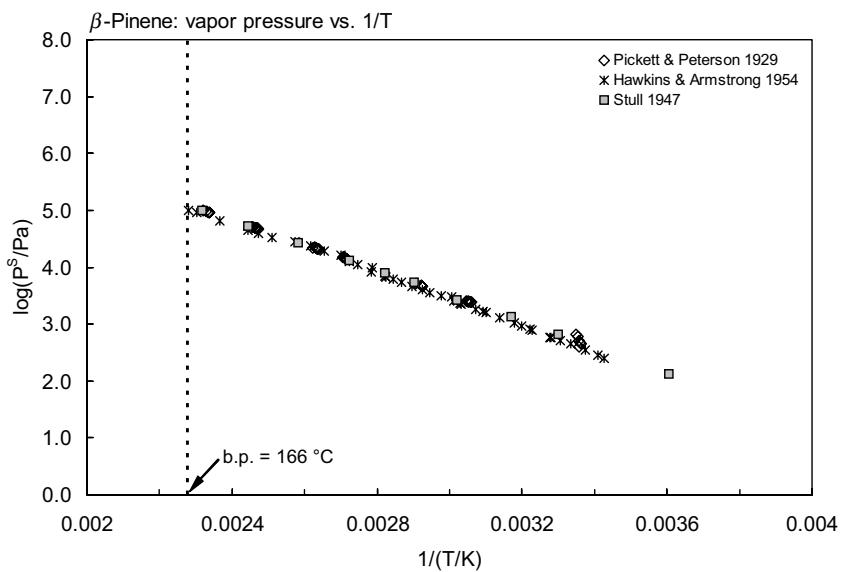
FIGURE 2.1.2.4.10.1 Logarithm of vapor pressure versus reciprocal temperature for β-pinene.

2.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 2.2.1
Summary of physical properties of aliphatic and cyclic hydrocarbons

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p.°C	b.p.°C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V_M cm³/mol MW/ρ at 20°C	Le Bas
Alkanes:									
Isobutane (2-Methylpropane)	75-28-5	C_4H_{10}	58.122	−159.4	−11.73	1	0.5571	104.33	96.2
2,2-Dimethylpropane (Neopentane)	463-82–1	C_5H_{12}	72.149	−16.4	9.48	1	0.5910	122.08	118.4
n-Butane	106-97-8	C_4H_{10}	58.122	−138.3	−0.5	1	0.5786	100.45	96.2
2-Methylbutane (Isopentane)	78-78-4	C_5H_{12}	72.149	−159.77	27.88	1	0.6193	116.50	118.4
2,2-Dimethylbutane	75-83-2	C_6H_{14}	86.175	−98.8	49.73	1	0.6492	132.74	140.6
2,3-Dimethylbutane	79-29-8	C_6H_{14}	86.175	−128.10	57.93	1	0.6616	130.25	140.6
2,2,3-Trimethylbutane	464-06-2	C_7H_{16}	100.202	−24.6	80.86	1	0.6901	145.20	162.8
n-Pentane	109-66-0	C_5H_{12}	72.149	−129.67	36.06	1	0.6262	115.22	118.4
2-Methylpentane (Isohexane)	107-83-5	C_6H_{14}	86.175	−153.6	60.26	1	0.6322	136.31	140.6
3-Methylpentane	96-14-0	C_6H_{14}	86.175	−162.90	63.27	1	0.66431	129.72	140.6
2,2-Dimethylpentane	590-35-2	C_7H_{16}	100.202	−123.7	79.2	1	0.6739	148.69	162.8
2,4-Dimethylpentane	108-08-7	C_7H_{16}	100.202	−119.5	80.49	1	0.6727	148.95	162.8
3,3-Dimethylpentane	562-49-2	C_7H_{16}	100.202	−134.4	86.06	1	0.6933	144.53	162.8
2,2,4-Trimethylpentane (Isooctane)	540-84-1	C_8H_{18}	114.229	−107.3	99.22	1	0.6919	165.09	185.0
2,3,4-Trimethylpentane	565-75-3	C_8H_{18}	114.229	−109.2	113.5	1	0.7191	158.85	185.0
n-Hexane	110-54-3	C_6H_{14}	86.175	−95.35	68.73	1	0.6593	130.71	140.6
2-Methylhexane (Isoheptane)	591-76-4	C_7H_{16}	100.202	−118.2	90.04	1	0.6786	147.66	162.8
3-Methylhexane	589-34-4	C_7H_{16}	100.202	−119.4	92	1	0.6871	145.83	162.8
2,2,5-Trimethylhexane	3522-94-9	C_9H_{20}	128.255	−105.7	124.09	1	0.7072	181.36	207.2
n-Heptane	142-82-5	C_7H_{16}	100.202	−90.55	98.4	1	0.6837	146.56	162.8
2-Methylheptane	592-27-8	C_8H_{18}	114.229	−109.02	117.66	1	0.698	163.65	185.0
3-Methylheptane	589-81-1	C_8H_{18}	114.229	−120.48	118.9	1	0.7075	161.45	185.0
n-Octane	111-65-9	C_8H_{18}	114.229	−56.82	125.67	1	0.70256	162.59	185.0
4-Methyloctane	2216-34-4	C_9H_{20}	128.255	−113.3	142.4	1	0.7199	178.16	207.2
n-Nonane	111-84-2	C_9H_{20}	128.255	−53.46	150.82	1	0.7177	178.70	207.2
n-Decane	124-18-5	$C_{10}H_{22}$	142.282	−29.6	174.15	1	0.7301	194.88	229.4
n-Undecane	1120-21-4	$C_{11}H_{24}$	156.309	−25.5	195.9	1	0.7402	211.17	251.6
n-Dodecane	112-40-3	$C_{12}H_{26}$	170.334	−9.57	216.32	1	0.7487	227.51	273.8
n-Tridecane	629-50-5	$C_{13}H_{28}$	184.361	−5.4	235.47	1	0.7564	243.73	296.0

(Continued)

TABLE 2.2.1 (*Continued*)

Compound	CAS no.	Molecular formula	Molecular weight, MWg/mol	m.p.°C	b.p.°C	Fugacity ratio, F at 25°C*	Density, ρg/cm³ at 20°C	Molar volume, V_M cm³/mol	
								MW/ρ at 20°C	Le Bas
n-Tetradecane	629-59-4	$C_{14}H_{30}$	198.388	5.82	253.58	1	0.7628	260.08	318.2
n-Pentadecane	629-62-9	$C_{15}H_{32}$	212.415	9.95	270.6	1	0.7685	276.40	340.4
n-Hexadecane	544-76-3	$C_{16}H_{34}$	226.441	18.12	286.86	1	0.77344	292.77	362.6
n-Heptadecane	629-78-7	$C_{17}H_{36}$	240.468	22.0	302.0	1	0.7780	309.08	384.8
n-Octadecane	593-45-3	$C_{18}H_{38}$	254.495	28.2	316.3	0.930	0.7819	325.48	407.0
n-Eicosane	112-95-8	$C_{20}H_{42}$	282.547	36.6	343	0.769	0.7887	358.24	451.4
n-Tetracosane	646-31-1	$C_{24}H_{50}$	338.654	50.4	391.3	0.563	0.7991	423.79	540.2
n-Hexacosane	630-01-3	$C_{26}H_{54}$	366.707	56.1	412.2	0.495	0.8032	456.56	584.6
Cycloalkanes:									
Cyclopentane	287-92-3	C_5H_{10}	70.133	–93.4	49.3	1	0.7454	94.09	99.5
Methylcyclopentane	96-37-7	C_6H_{12}	84.159	–142.42	71.8	1	0.7487	112.41	121.7
1,1,3-Trimethylcyclopentane	4516-69-2	C_8H_{16}	112.213	–142.4	104.9	1	0.7483	149.96	166.1
Propylcyclopentane	2040-96-2	C_8H_{16}	112.213	–117.3	131	1	0.7763	144.55	166.1
Pentylcyclopentane	3741-00-2	$C_{10}H_{20}$	140.266	–83	180	1	0.7912	177.28	210.5
Cyclohexane	110-82-7	C_6H_{12}	84.159	6.59	80.73	1	0.7786	108.09	118.2
Methylcyclohexane	108-87-2	C_7H_{14}	98.186	–126.6	100.93	1	0.7694	127.61	140.4
1,2-*cis*-Dimethylcyclohexane	2207-01-4	C_8H_{16}	112.213	–49.8	129.8	1	0.7963	140.92	162.6
1,4-*trans*-Dimethylcyclohexane	2207-04-7	C_8H_{16}	112.213	–36.93	119.4	1	0.7626	147.15	162.6
1,1,3-Trimethylcyclohexane	3073-66-3	C_9H_{18}	126.239	–65.7	136.6	1	0.7664	165.72	184.8
Ethylcyclohexane	1678-91-7	C_8H_{16}	112.213	–111.3	131.9	1	0.7880	142.40	162.6
Cycloheptane	291-64-5	C_7H_{14}	98.186	–8.46	118.4	1	0.8098	121.25	136.4
Cyclooctane	292-64-8	C_8H_{16}	112.213	14.59	149	1	0.8340	134.55	154.1
cis-Decalin	493-01-6	$C_{10}H_{18}$	138.250	–42.9	195.8	1	0.8931	154.80	184.6
trans-Decalin	493-02-7	$C_{10}H_{18}$	138.250	–30.4	187.3	1	0.8662	159.60	184.6
Alkenes:									
2-Methylpropene	115-11-7	C_4H_8	56.107	–140.7	–6.9	1	0.5942	94.42	88.8
1-Butene	106-98-9	C_4H_8	56.107	–185.34	–6.26	1	0.5951	94.28	88.8
2-Methyl-1-butene	563-46-2	C_5H_{10}	70.133	–137.53	31.2	1	0.6504	107.83	111.0
3-Methyl-1-butene	563-45-1	C_5H_{10}	70.133	–168.43	20.1	1	0.6272	111.82	111.0
2-Methyl-2-butene	513-35-9	C_5H_{10}	70.133	–133.72	38.56	1	0.6623	105.89	111.0
1-Pentene	109-67-1	C_5H_{10}	70.133	–165.12	29.96	1	0.6405	109.50	111.0
cis-2-Pentene	627-20-3	C_5H_{10}	70.133	–151.36	36.93	1	0.6556	106.98	111.0
2-Methyl-1-pentene	763-29-1	C_6H_{12}	84.159	–135.7	62.1	1	0.6799	123.78	133.2
4-Methyl-1-pentene	691-37-2	C_6H_{12}	84.159	–153.6	53.9	1	0.6642	126.71	133.2

1-Hexene	592-41-6	C_6H_{12}	84.159	–139.76	63.48	1	0.6732	125.01	133.2
1-Heptene	592-76-7	C_7H_{14}	98.186	–118.9	93.64	1	0.6970	140.87	155.4
1-Octene	111-66-0	C_8H_{16}	112.213	–101.7	121.29	1	0.7149	156.96	177.6
1-Nonene	124-11-8	C_9H_{18}	126.239	–81.3	146.9	1	0.7292	173.12	199.8
1-Decene	872-05-9	$C_{10}H_{20}$	140.266	–66.3	170.5	1	0.7408	189.34	222.0
Dienes:									
1,3-Butadiene	106-99-0	C_4H_6	54.091	–108.91	–4.41	1	0.6211	87.09	81.4
2-Methyl-1,3-butadiene (Isoprene)	78-79-5	C_5H_8	68.118	–145.9	34.0	1	0.6809	100.04	103.6
2,3-Dimethyl-1,3-butadiene	513-81-5	C_6H_{10}	82.143	–76	68.8	1	0.7267	113.04	125.8
1,4-Pentadiene	591-93-5	C_5H_8	68.118	–148.2	26	1	0.6608	103.08	103.6
1,5-Hexadiene	592-42-7	C_6H_{10}	82.143	–140.7	59.4	1	0.6923	118.65	125.8
1,6-Heptadiene	3070-53-9	C_7H_{12}	96.170	–129	90	1	0.714	134.69	148.0
Alkynes:									
1-Butyne	107-00-6	C_4H_6	54.091	–125.7	8.08	1	0.650	83.22	81.4
1-Pentyne	627-19-0	C_5H_8	68.118	–90	40.1	1	0.6901	98.71	103.6
1-Hexyne	693-02-7	C_6H_{10}	82.143	–131.9	71.3	1	0.7155	114.81	125.8
1-Heptyne	628-71-7	C_7H_{12}	96.170	–81	99.7	1	0.7328	131.24	148.0
1-Octyne	629–05–0	C_8H_{14}	110.197	–79.3	126.3	1	0.7461	147.70	170.2
1-Nonyne	3452–09–3	C_9H_{16}	124.223	–50	150.8	1	0.7568	164.14	192.4
Cycloalkenes:									
Cyclopentene	142-29-0	C_5H_8	68.118	–135.0	44.2	1	0.772	88.24	92.1
Cyclohexene	110-83-8	C_6H_{10}	82.143	–103.5	82.98	1	0.8110	101.29	110.8
1-Methylcyclohexene	591-49-1	C_7H_{12}	96.170	–120.4	110.3	1	0.8102	118.70	133.0
Cycloheptene	628-92-2	C_7H_{12}	96.170	–56	115	1	0.8228	116.88	129.0
cis-Cyclooctene	931-87-3	C_8H_{14}	110.197	–12	138	1	0.8472	130.07	146.7
trans-Cyclooctene	931-89-5	C_8H_{14}	110.197	–59	143	1	0.8483	129.90	146.7
1,4-Cyclohexadiene	628-41-1	C_6H_8	80.128	–49.2	85.5	1	0.8471	94.59	103.4
1,3,5-Cycloheptatriene	544-25-2	C_7H_8	92.139	–79.5	117	1	0.8875	103.82	114.2
d-Limonene	5989-27-5	$C_{10}H_{16}$	136.234	–74.0	178	1	0.8403	162.13	192.2
α-Pinene	80-56-8	$C_{10}H_{16}$	136.234	–64	156.2	1	0.8582	158.74	183.7
β-Pinene	127-91-3	$C_{10}H_{16}$	136.234	–61.5	166	1	0.8694	156.70	183.7

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 2.2.2
Summary of selected physical-chemical properties of aliphatic and cyclic hydrocarbons at 25°C

Compound	Vapor pressure		Solubility			log K_{ow}	Henry's law constant $H/(Pa \cdot m^3/mol)$
	P^S/Pa	P_L/Pa	$S/(g/m^3)$	$C^S/(mol/m^3)$	$C_L/(mol/m^3)$		calculated P/C
Alkanes:							
Isobutane (2-Methylpropane)	357000	357000	48.9	0.8413	0.8413	2.76	120435*
2,2-Dimethylpropane	172000	172000	33.2	0.4602	0.4602	3.11	220195*
n-Butane	243000	243000	61.4	1.0564	1.0564	2.90	95915*
2-Methylbutane (Isopentane)	91640	91640	47.8	0.6625	0.6625	2.30	138320
2,2-Dimethylbutane	42600	42600v	18.4	0.2135	0.2135	3.82	199515
2,3-Dimethylbutane	32010	32010	19.1	0.2216	0.2216	3.85	144422
2,2,3-Trimethylbutane	13652	13652	4.38	0.0437	0.0437		312320
n-Pentane	68400	68400	38.5	0.5336	0.5336	3.45	128180
2-Methylpentane (Isohexane)	28200	28200	13.8	0.1601	0.1601	2.80	176097
3-Methylpentane	25300	25300	12.8	0.1485	0.1485	3.60	170330
2,2-Dimethylpentane	14000	14000	4.4	0.0439	0.0439	3.10	318825
2,4-Dimethylpentane	13100	13100	4.06	0.0405	0.0405	3.10	323312
3,3-Dimethylpentane	10940	10940	5.94	0.0593	0.0593		184550
2,2,4-Trimethylpentane (Isooctane)	6560	6560	2.44	0.0214	0.0214		307110
2,3,4-Trimethylpentane	3600	3600	2.0	0.0119	0.0119		205614
n-Hexane	20200	20200	9.5	0.1102	0.1102	4.11	183235
2-Methylhexane (Isoheptane)	8780	8780	2.54	0.0253	0.0253		346370
3-Methylhexane	8210	8210	3.3	0.0329	0.0329		249290
2,2,5-Trimethylhexane	2210	2210	1.15	0.0090	0.0090	4.50	246472
n-Heptane	6110	6110	2.93	0.0292	0.0292	5.00	208955
2-Methylheptane	2600	2600	0.85	0.00744	0.0074		349410
n-Octane	1800	1800	0.66	0.005778	0.0058	5.15	311536
n-Nonane	571	571	0.22	0.001715	0.0017	5.65	332880
n-Decane	175	175	0.052	0.000365	0.00037	6.25	478840
n-Undecane	52.2	52.2	0.004	0.000026	0.000026		2039835
n-Dodecane	18.02	18.02	0.0037	0.000022	0.000022	6.80	829570
n-Tridecane	6.682	6.682					
n-Tetradecane	1.804	1.804				8.00	
n-Hexadecane	0.191	0.191					
n-Heptadecane	0.0615	0.0615					
n-Octadecane	0.02	0.019					

n-Eicosane	0.00209	0.00161					
Cycloalkanes:							
Cyclopentane	42400	42400	166	2.3669	2.3669	3.00	17915
Methylcyclopentane	18300	18300	43	0.5109	0.5109	3.37	35815
1,1,3-Trimethylcyclopentane	5300	5300	3.73	0.0332	0.0332		159440
Propylcyclopentane	1640	1640	2.04	0.0182	0.0182		90210
Pentylcyclopentane	152	152	0.115	0.0008	0.0008		185395
Cyclohexane	13014	13014	58	0.6892	0.6892	3.44	18885
Methylcyclohexane	6180	6180	15.1	0.1538	0.1538	3.88	40185
1,2-*cis*-Dimethylcyclohexane	1930	1930	6	0.0535	0.0535		36095
1,4-*trans*-Dimethylcyclohexane	3020	3020	3.84	0.0342	0.0342		88250
1,1,3-Trimethylcyclohexane	1480	1480	1.77	0.0140	0.0140		105560
Cycloheptane	2924	2924	23.5	0.2393	0.2393		12220
Cyclooctane	748	748	5.80	0.0517	0.0517	4.45	14470
Alkenes:							
2-Methylpropene	304000	304000	263	4.6875	4.6875		21620*
1-Butene	297000	297000	222	3.9567	3.9567		25610*
2-Methyl-1-butene	81330	81330					
3-Methyl-1-butene	120000	120000	130	1.8536	1.8536		54670*
2-Methyl-2-butene	62410	62410	325	4.634	4.634		13470
1-Pentene	85000	85000	148	2.1103	2.1103	2.20	40280
cis-2-Pentene	66000	66000				2.20	
2-Methyl-1-pentene	26000	26000	78	0.9268	0.9268		28050
4-Methyl-1-pentene	36100	36100	48	0.5703	0.5703	2.50	63295
1-Hexene	24800	24800	50	0.5941	0.5941	3.39	41743
1-Heptene	7510	7510	18.3	0.1864	0.1864	3.99	40295
1-Octene	2320	2320	2.7	0.0241	0.0241	4.57	96420
1-Nonene	712	712	1.12	0.0089	0.0089	5.15	80250
1-Decene	218	218					
Dienes:							
1,3-Butadiene	281000	281000	735	13.588	13.588	1.99	7458*
2-Methyl-1,3-butadiene (Isoprene)	73300	73300	642	9.4248	9.4248		7780
2,3-Dimethyl-1,3-butadiene	20160	20160	327	3.9809	3.9809		5065
1,4-Pentadiene	98000	98000	558	8.1917	8.1917	2.48	11965
1,5-Hexadiene	29690	29690	169	2.0574	2.0574	2.75	14430
1,6-Heptadiene			44	0.4575	0.4575		

(*Continued*)

TABLE 2.2.2 (*Continued*)

Compound	Vapor pressure		Solubility			log K_{ow}	Henry's law constant H/(Pa·m³/mol) calculated P/C
	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)		
Alkynes:							
1-Butyne	188000	188000	2870	53.059	53.059		1910*
1-Pentyne	57600	57600	1570	23.048	23.048	1.98	2500
1-Hexyne	18140	18140	360	4.3830	4.3830	2.73	4140
1-Heptyne	7500	7000	94	0.9774	0.9774	2.98	7675
1-Octyne	1715	1715	24	0.2178	0.2178		7875
1-Nonyne			7.2	0.0580	0.0580		
Cycloalkenes:							
Cyclopentene	50710	50706	535	7.8540	7.8540	2.48	6455
Cyclohexene	11850	11850	213	2.5928	2.5928	2.86	4570
1-Methylcyclohexene	4689	4689	52	0.5407	0.5407		8670
Cycloheptene	2670	2670	66	0.6863	0.6863		3890
Cyclooctene	1010	1010	22.9	0.2078	0.2078	2.47	4860
1,4-Cyclohexadiene	9009	9009	800	9.9840	9.9840		902
1,3,5-Cycloheptatriene	3140	3140	620	7.7376	7.7376	2.63	467
d-Limonene	270	270	13.8	0.1013	0.1013		2665
α-Pinene	582	582					
β-Pinene	395	395					

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H/(Pa·m³/mol) = 101325 Pa/C^S mol/m³.

TABLE 2.2.3
Suggested half-life classes of hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Alkanes:				
n-Pentane	2	5	6	7
n-Hexane	2	5	6	7
n-Octane	2	5	6	7
n-Decane	2	5	6	7
n-Dodecane	2	5	6	7
Cycloalkanes:				
Cyclopentane	2	5	5	6
Methylcyclopentane	2	5	5	6
Cyclohexane	2	5	5	6
Methylcyclohexane	2	5	5	6
Cyclooctane	2	5	5	6
Alkenes:				
1-Pentene	1	4	5	6
1-Octene	1	4	5	6
1,3-Butadiene	1	4	5	6
1,4-Pentadiene	1	4	5	6
Alkynes:				
1-Hexyne	1	4	5	6
Cycloalkenes:				
Cyclopentene	1	4	5	6
Cyclohexene	1	4	5	6

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	55000 (~ 6 years)	> 30,000
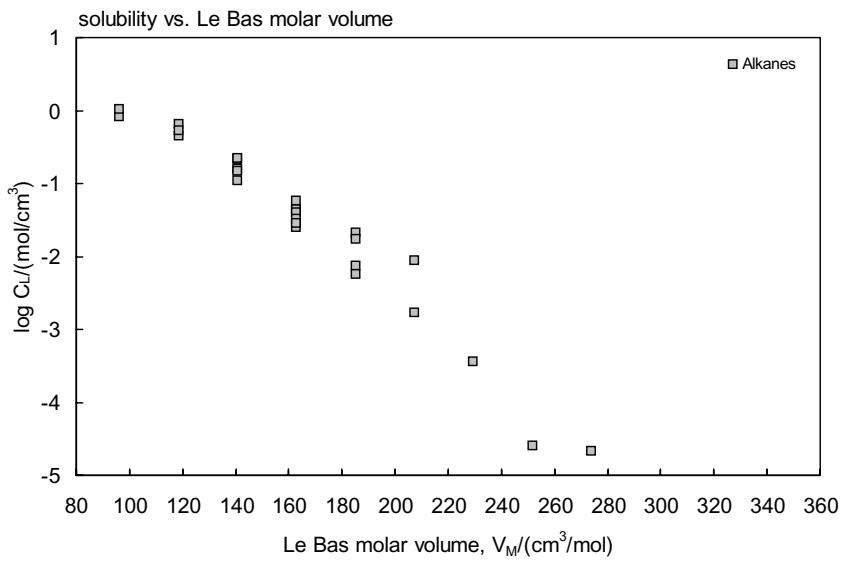
FIGURE 2.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.
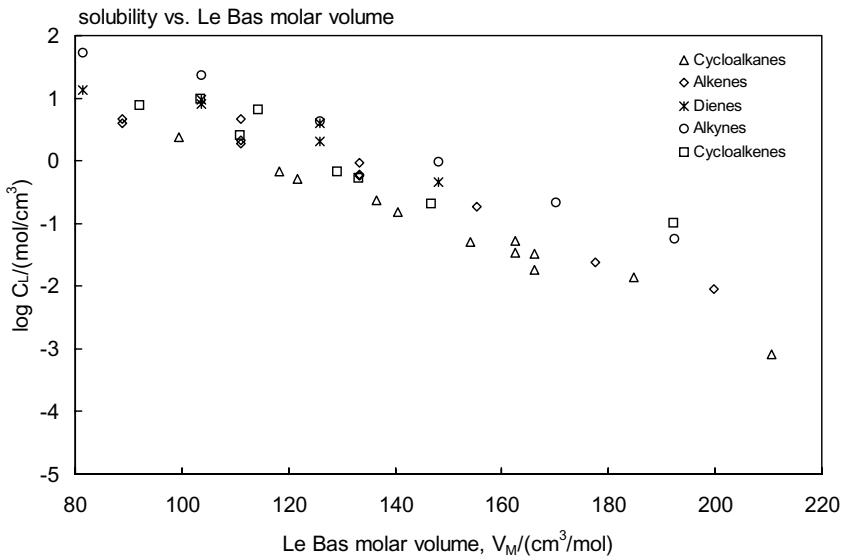

FIGURE 2.2.2 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.
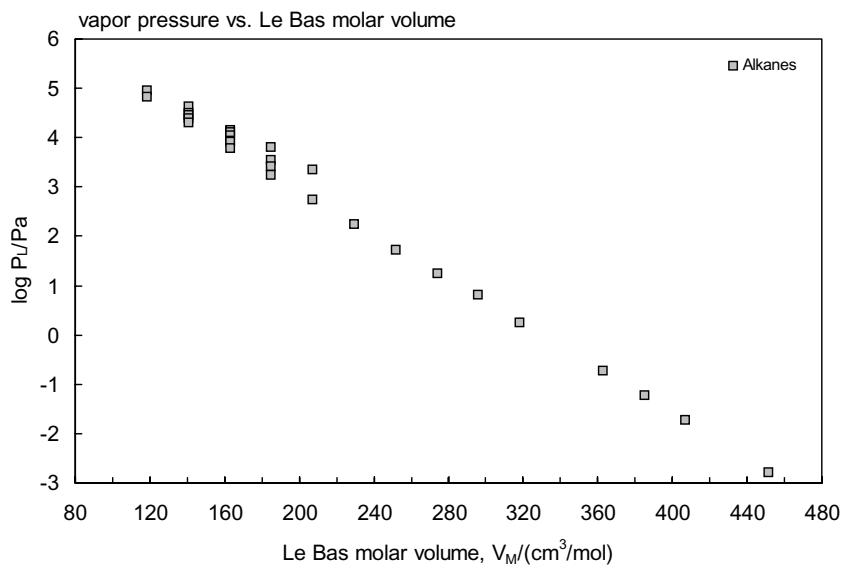
FIGURE 2.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.
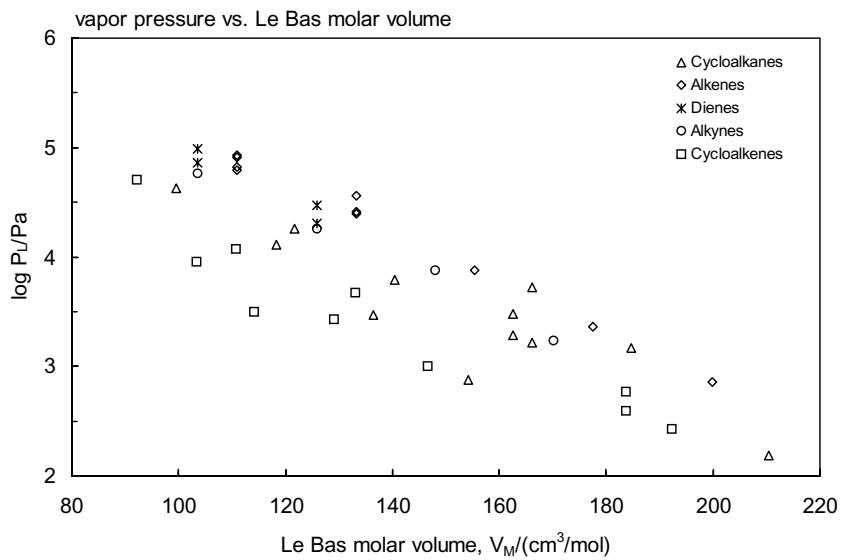

FIGURE 2.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.
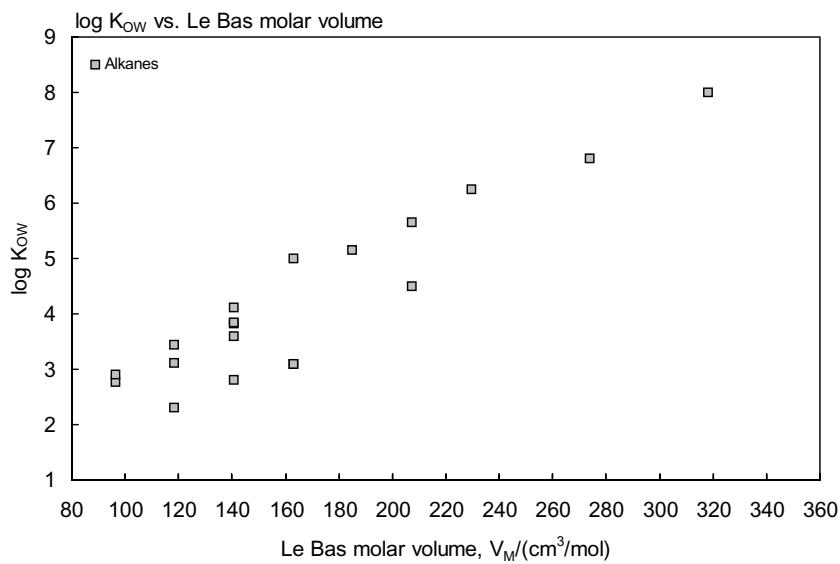
FIGURE 2.2.5 Octanol-water partition coefficient versus Le Bas molar volume for alkanes.
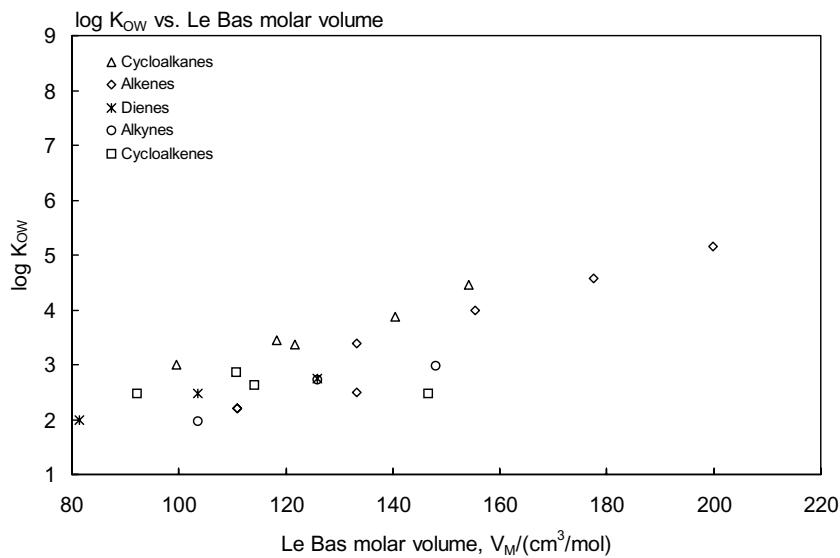

FIGURE 2.2.6 Octanol-water partition coefficient versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.
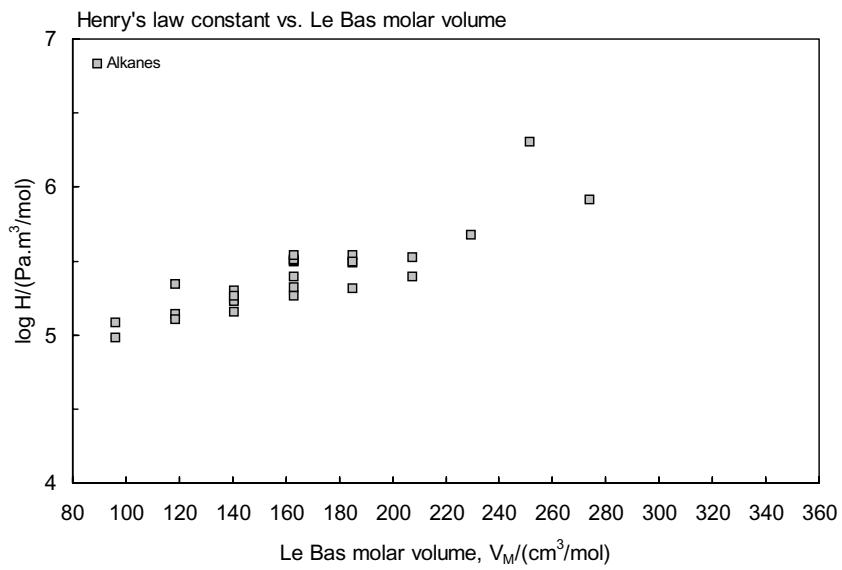
**FIGURE 2.2.7** Henry's law constant versus Le Bas molar volume for alkanes.
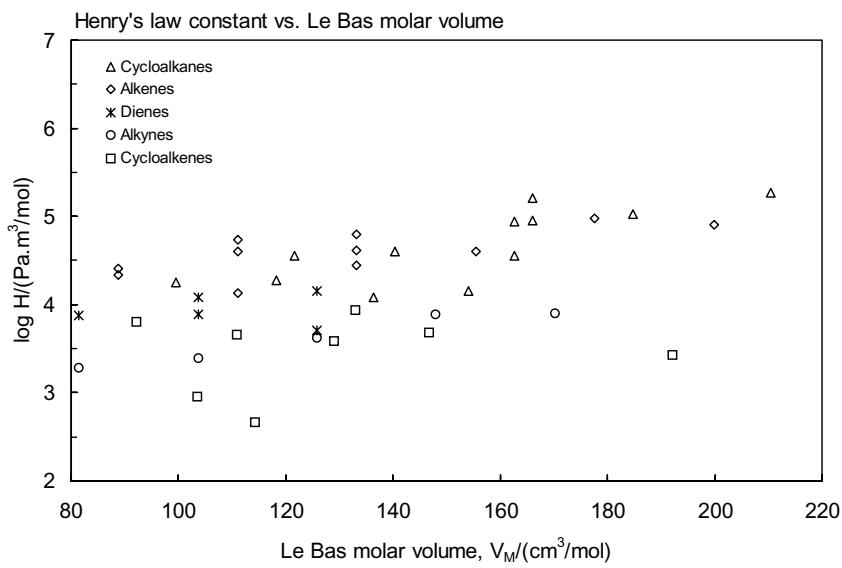
FIGURE 2.2.8 Henry's law constant versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.
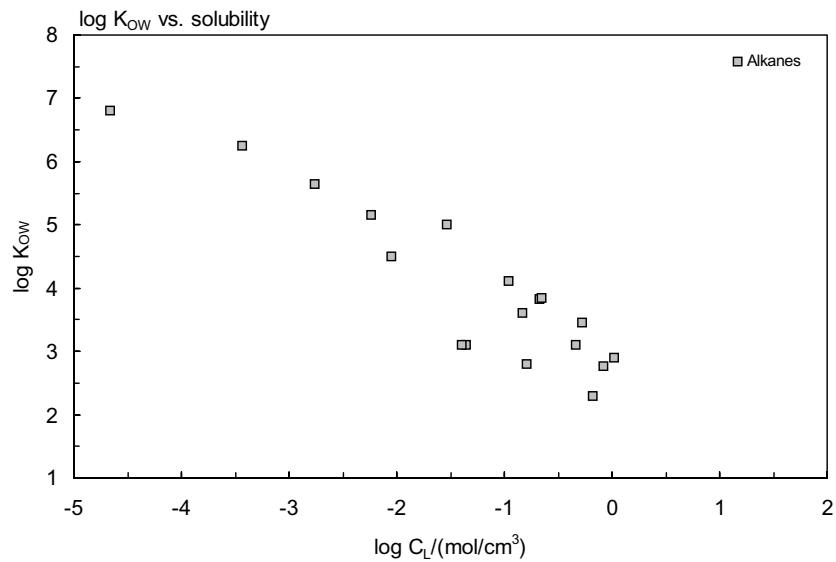
FIGURE 2.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alkanes.
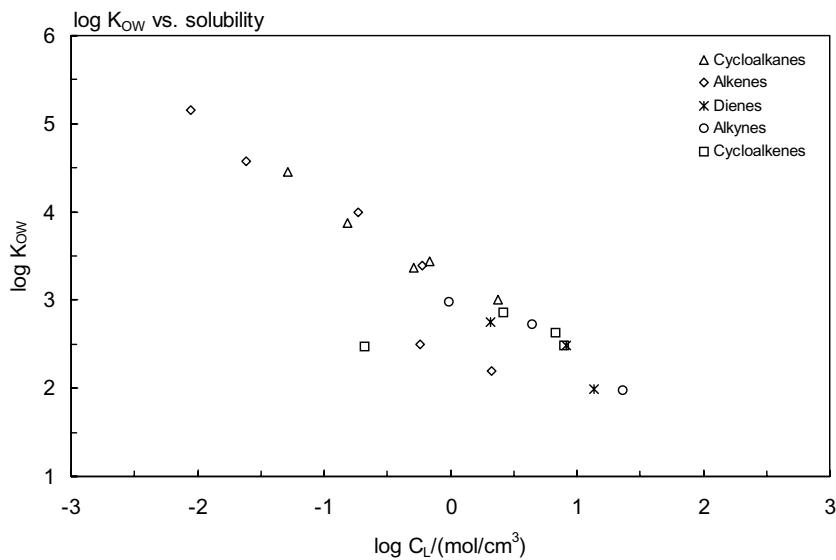

FIGURE 2.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aliphatic and cyclic hydrocarbons.

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